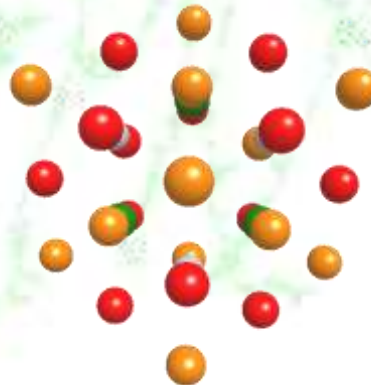
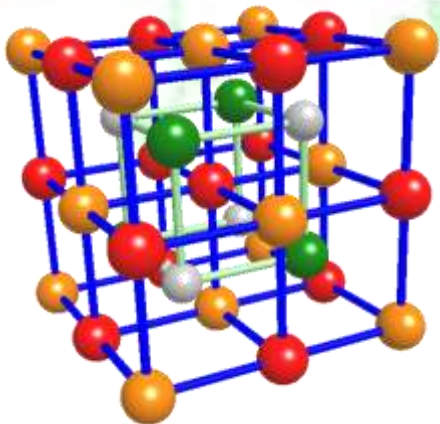


Ion beam analysis of Fe-based Heusler alloys/Ge hetero-epitaxial interfaces toward spin transistors

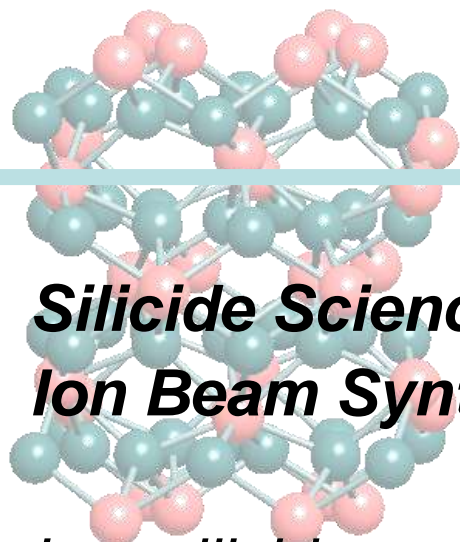
Y. Maeda

*Department of Computer Science and Electronics,
Kyushu Institute of Technology, Japan*

Advanced Science Research Center Japan Atomic Energy Agency



Our Research

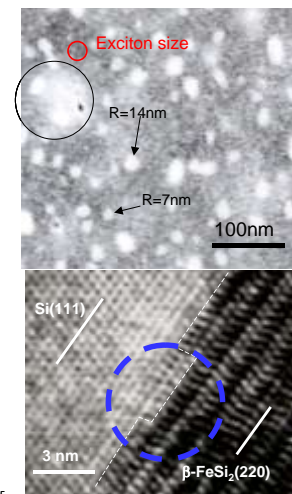
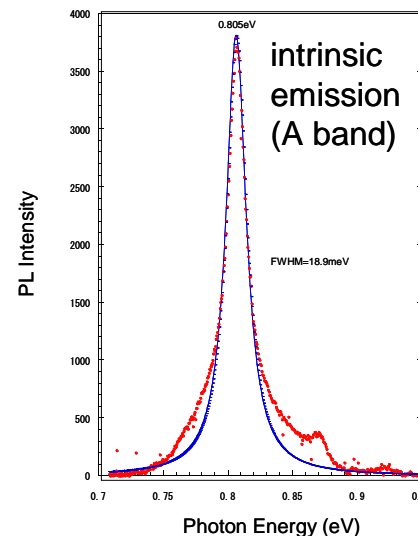
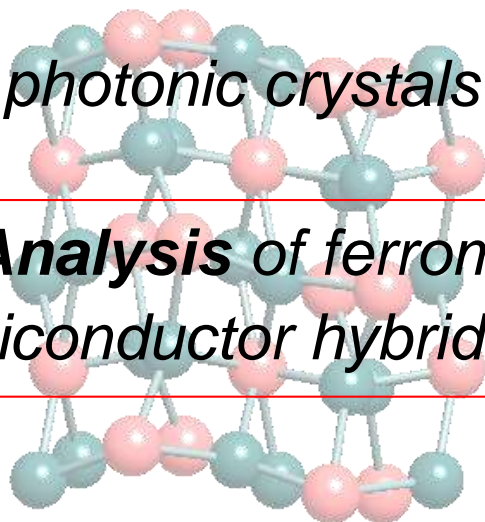


Silicide Science and Technology ***Ion Beam Synthesis of iron silicides***

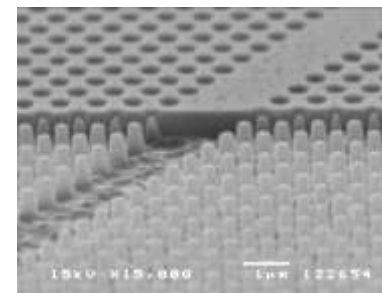
Iron silicide nanostructures for light emitter

Iron silicide photonic crystals

Ion Beam Analysis of ferromagnetic silicide/semiconductor hybrid structure



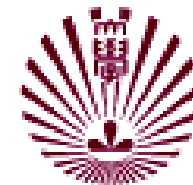
Photonic crystals
 β -FeSi₂, Fe₃Si



Collaborator



*Prof. M. Miyao, Prof. K. Hamaya, Prof. T. Sadoh
Kyushu University,
on MBE of ferromagnetic alloy films on semiconductors*



*Dr. M. Narumi, Dr. S. Sakai, Dr. K. Takahashi
Japan Atomic Energy Agency (JAEA)
on Ion beam analysis and development of beam lines
toward low temperature ion channeling experiments*



*Students graduated from Maeda Laboratory,
at Kyoto University, on RBS measurements.*



*Prof. Y. Terai, Dr. Y. Ando, Osaka University
on characterization of films*



Outline



1. Motivation

Ion Beam Analysis of materials for Spintronics.

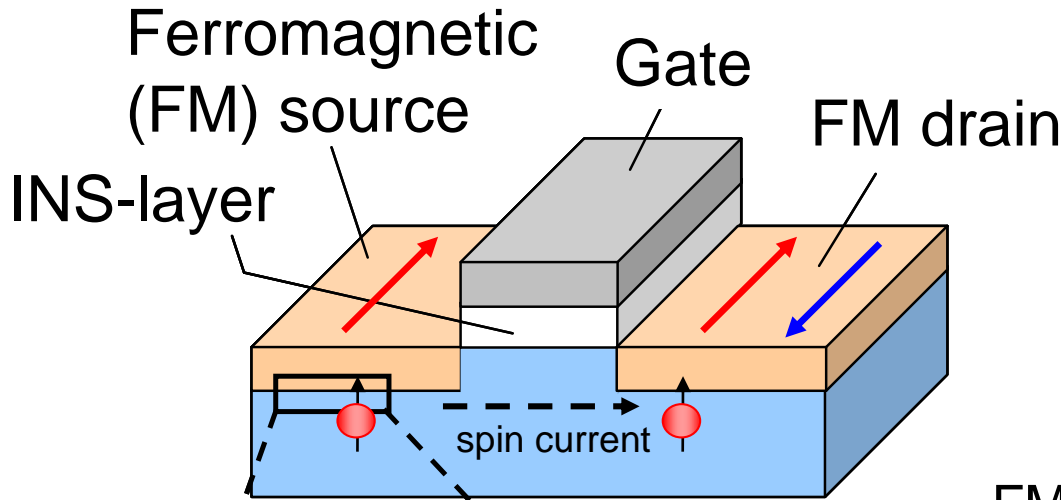
2. Ion Channeling and its application to

quantitative evaluation of disordering of some Heusler alloy films epitaxially grown on Ge(111).

3. Topic : Spin injection behavior related to quality of epitaxial growth of ferromagnetic (FM) Heusler alloy films Fe_3Si on Si(111).

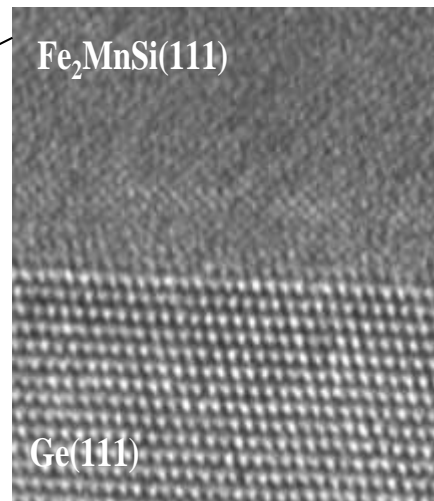
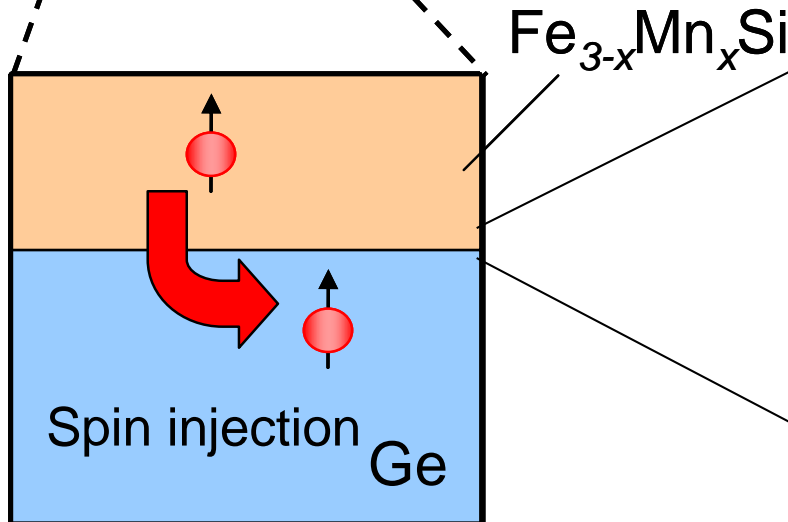
4. Conclusions

One of Goals of Spintronics, *Spin FET*



Spin-FET has a same device structure as MOSFET. We expect it on very high frequency operation and very low consuming power.

FM source epitaxially grown on Ge(111)



High quality heteroepitaxial interface realized by low temperature MBE technique.

K. Ueda et al: Appl. Phys. Lett. 93, (2008) 112108-1-3.

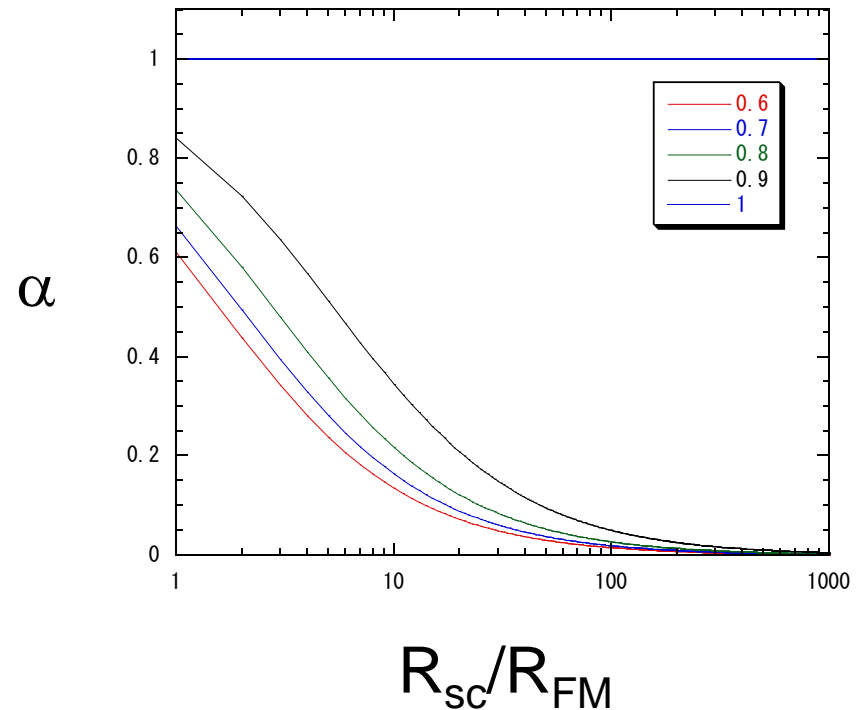
Efficiency of Spin Injection from FM into SC

$$\alpha = P_{\text{SC}} / P_{\text{FM}}$$
$$= \frac{1}{1 + \left(1 - P_{\text{FM}}^2\right) \left(\frac{R_{\text{SC}}}{R_{\text{FM}}}\right)}$$

P_{FM} : Spin polarity of FM

R_{SC} : Electrical resistivity of SC

R_{F} : Electrical resistivity of FM



In usual case, $R_{\text{SC}} \gg R_{\text{F}}$, so that $\alpha \ll 1$

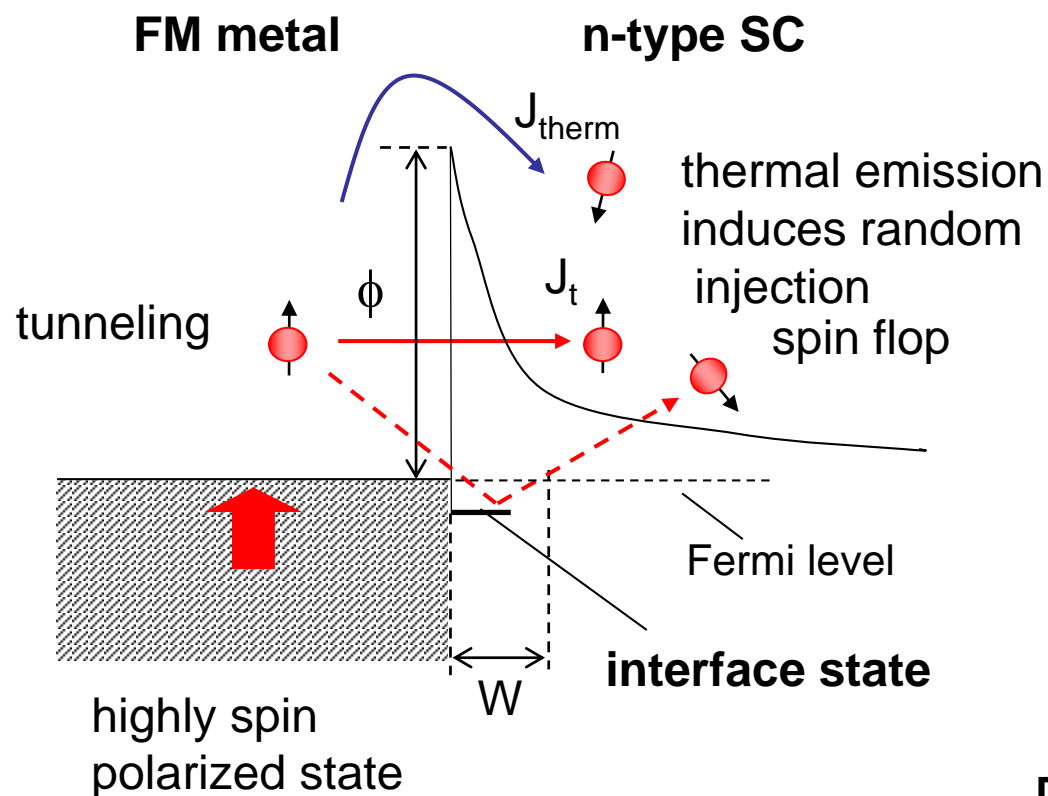
that is, Resistivity gap problem,

we have to overcome it for Spintronics.

Possible solutions

- Using *half metallic FM material* as an electrodes such as Fe_2MnSi etc.
(if possible, the problem remains.)
- Using Magnetic SC with highly polarized spin states. (in future, possible?)
- Using spin injection by **electron tunneling through a Schottky barrier. (Actually promising)**

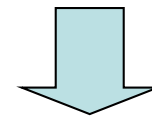
Spin injection by electron tunneling through Schottky barrier



Scheme of spin injection by electron tunneling through a Schottoky barrier

Conditions for Spin injection

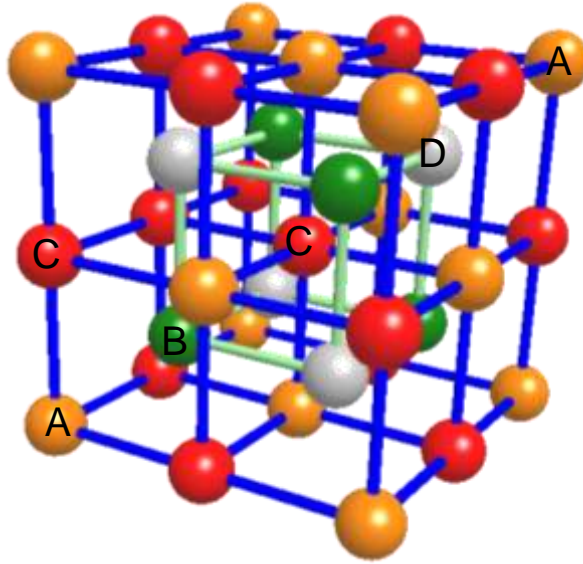
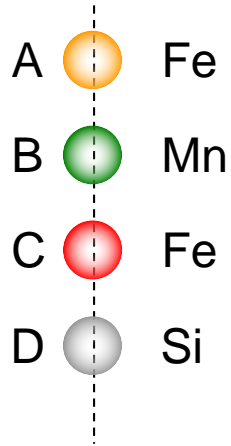
We need thinner barrier width enough to cause electron tunneling and higher barrier height enough to prevent thermal emission.



Delta dope technology and **Reduction of interface states by high quality MBE**

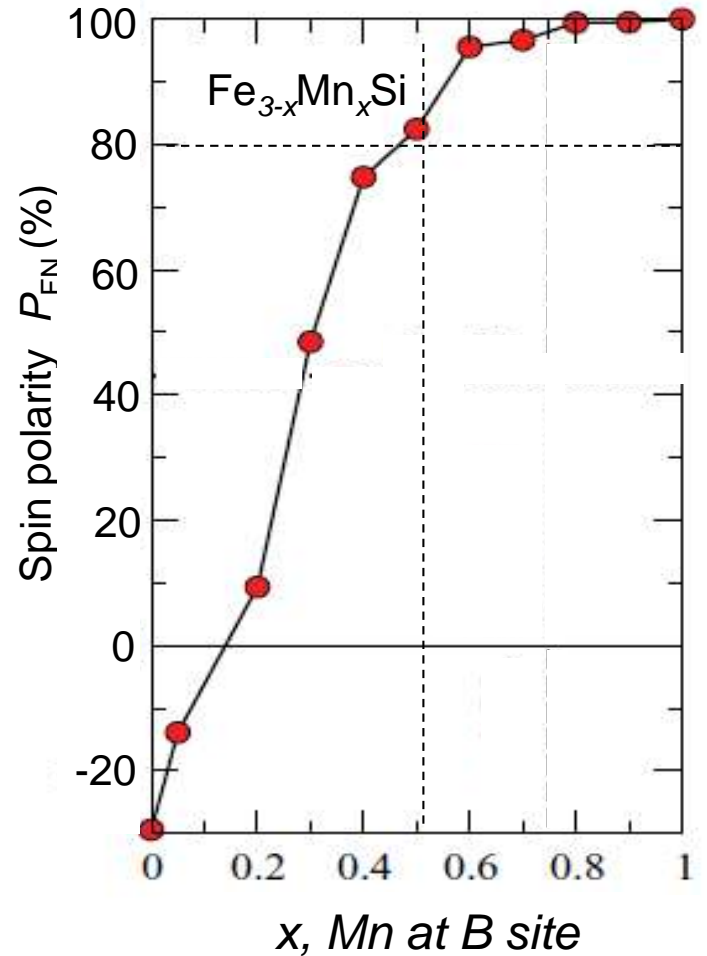
$\text{Fe}_{3-x}\text{Mn}_x\text{Si}$ (FMS) : Spin polarization

atomic row along
 $\langle 111 \rangle$



$L2_1$ type Heusler alloy
with ordered lattice Fe_2MnSi

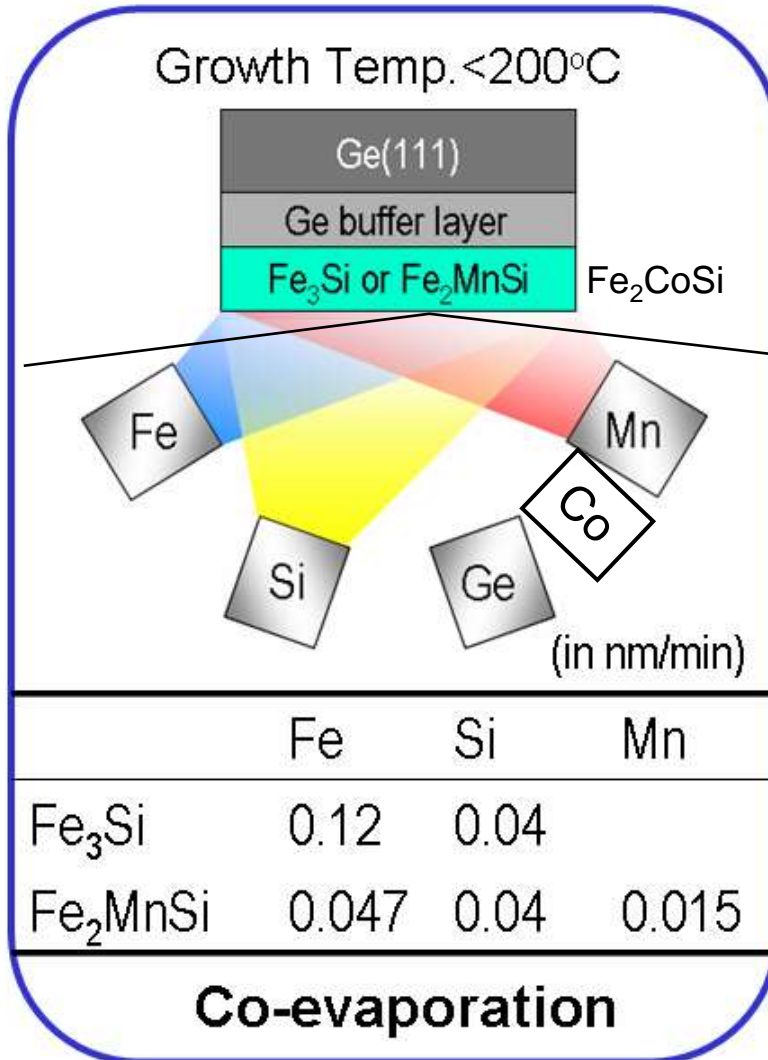
Stoichiometric Fe_2MnSi is estimated to be half metallic. Mn occupation at the B site affects spin polarization as shown in right figure.



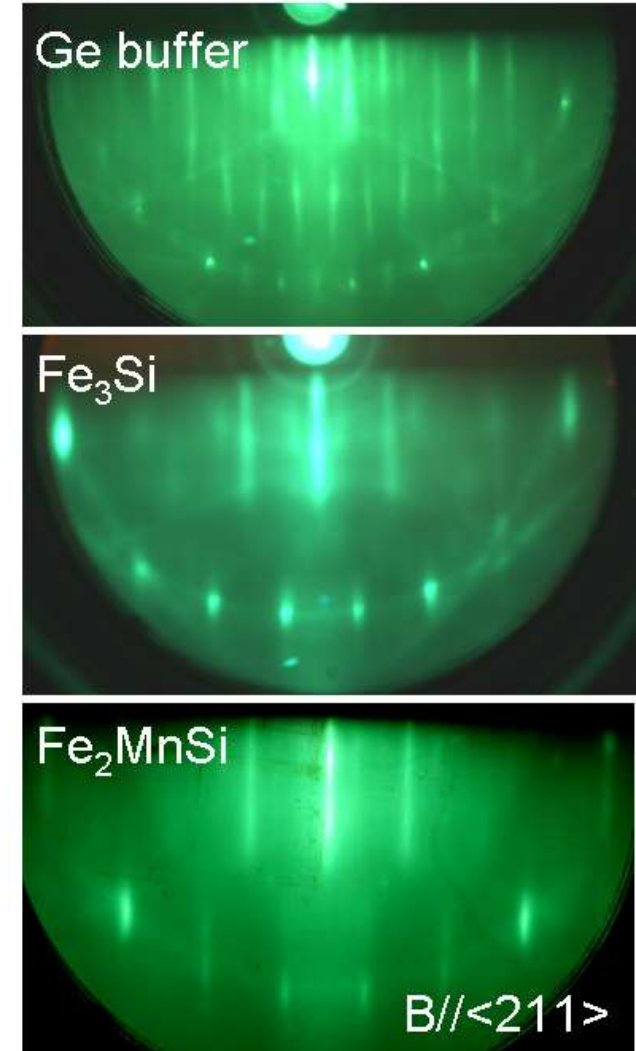
Low temperature MBE realized High quality Epitaxy

Low Temperature MBE

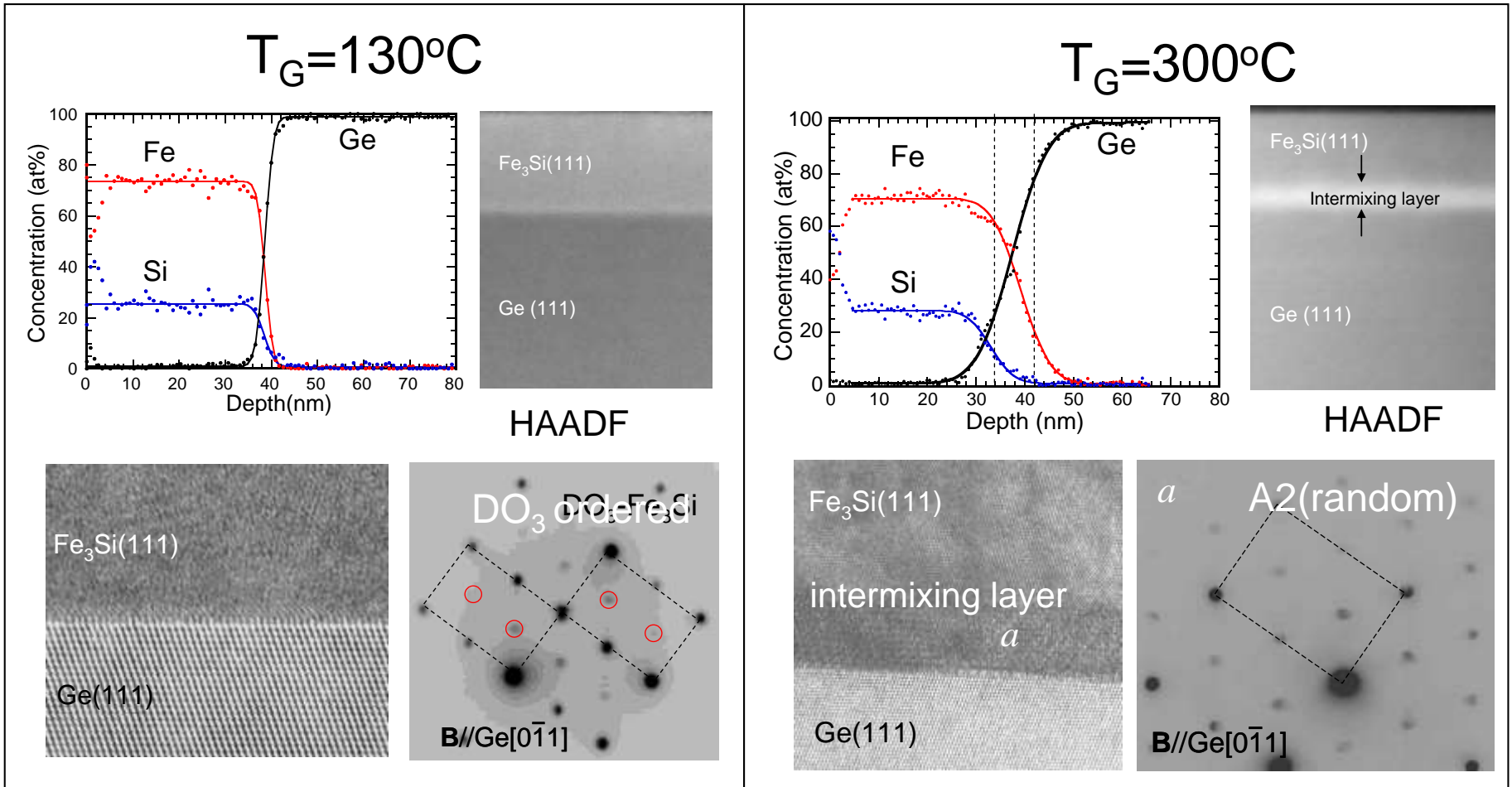
RHEED Patterns



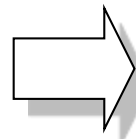
RHEED



Growth temperature T_G is crucial for high quality epitaxy of FM F_3Si/Ge



Low T_G is much better, we can prevent active interdiffusion between FM and Ge substrates and keep a DO_3 ordered lattice during growth.

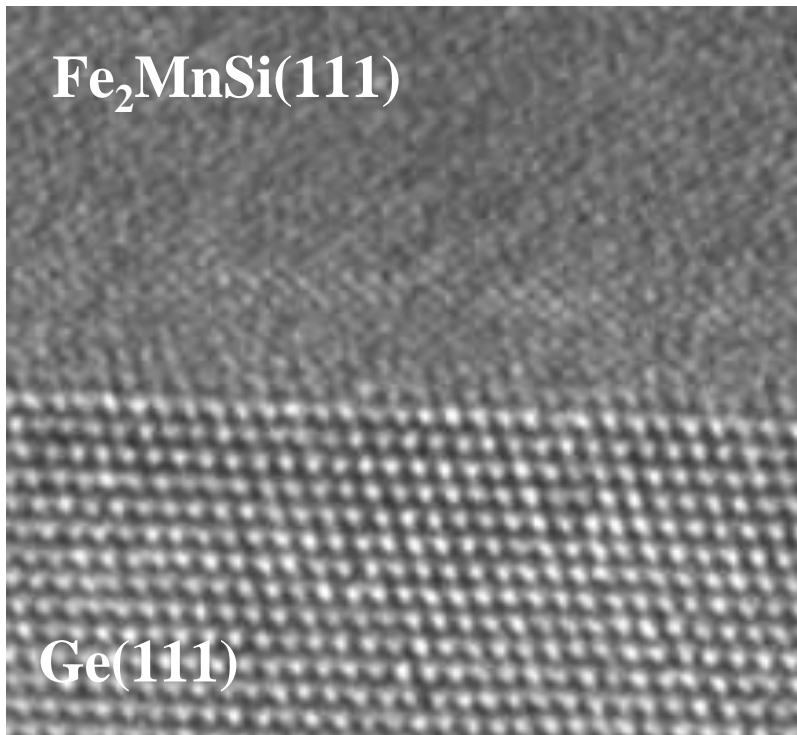


Low temperature MBE technique

XTEM, SAD observations of Fe₂MnSi(111)/Ge(111)

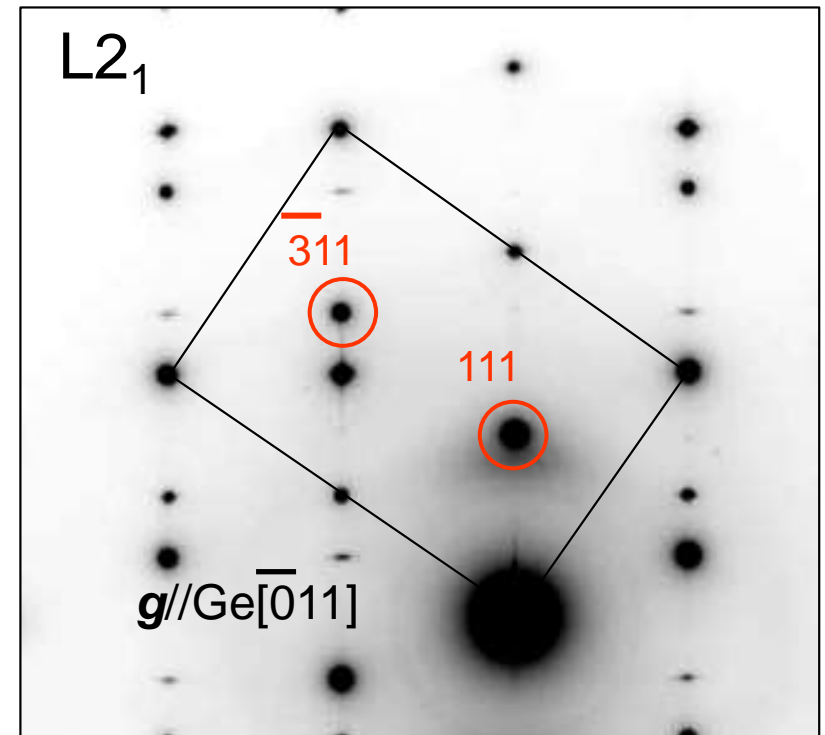
XTEM image

Fe₂MnSi(111)//Ge(111)



SAD pattern

Fe₂MnSi<111>//Ge<111>



○ L₂₁ super lattice reflection

K. Ueda et al: *Appl. Phys. Lett.* 93, (2008) 112108-1-3.

XTEM brings direct information of epitaxial interfaces, however, dose not teach the in-plane information at spin injection interfaces to us.

2.

**Introduction to Ion Channeling
and its application to Quantitative analysis
of disordering of some Heusler alloy films
epitaxially grown on Ge(111).**

Kinds of IBA

RBS

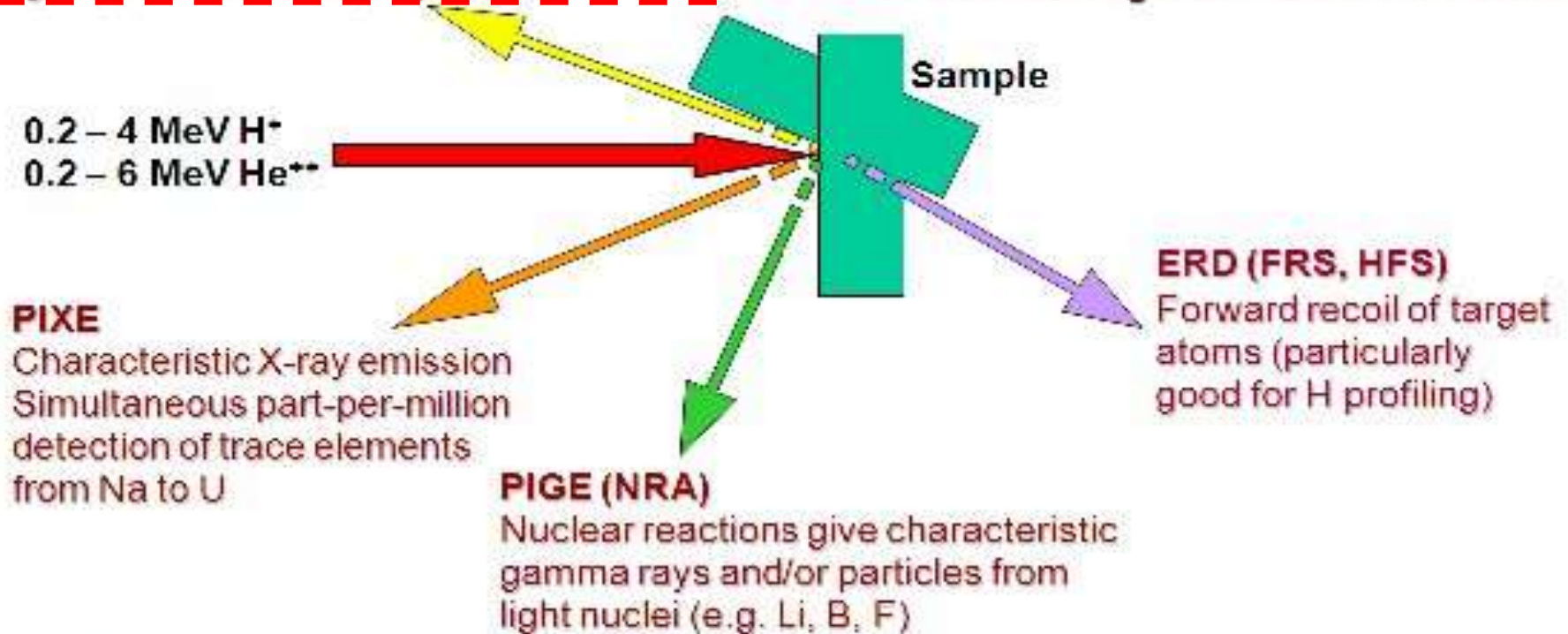
Protons or He particles are elastically scattered from the target nuclei: the scattered particles are energy analysed, giving elemental depth profiles

OTHER TECHNIQUES

IBIL: ion beam induced luminescence

IBIC: ion beam induced current

STIM: scanning transmission ion microscopy

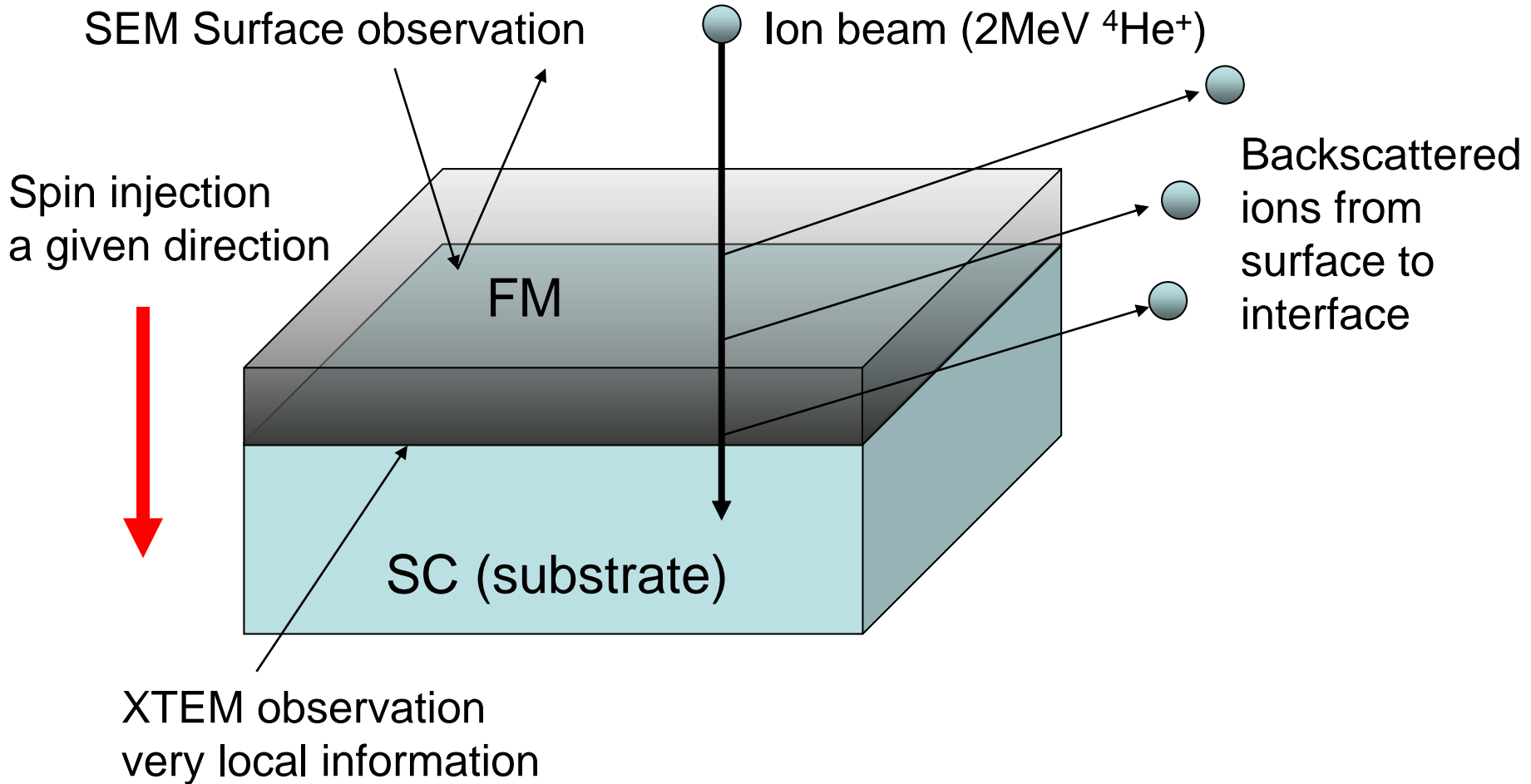


Ion Beam Analysis involves the use of an energetic ion beam to probe the surface of a material to reveal details of the elemental and structural details of it make up.

cited from SCRIBA, University of Surrey

Why do we need IBA?

IBA: Ion Beam Analysis



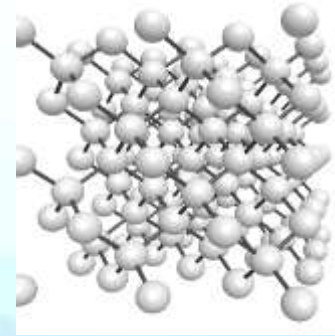
Using IBA, we can obtain not only atomic information at a tentative spin injection interface but also information from surface and the interface under nondestructive sample conditions.

Advantages of IBA

- Nondestructive
under low dose of incident ions
- element resolution analysis
- Depth analysis
- Average information at analyzing macro-area
- Usage of channeling techniques for
analysis of depth distribution of disorder,
location of impurity

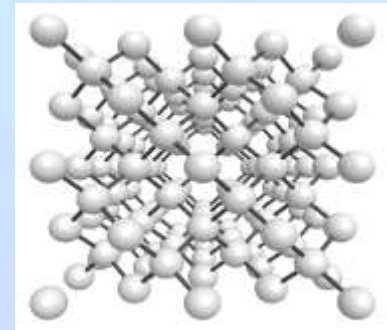
Rutherford Backscattering

- **Random scattering** gives information of depth distribution of elements involved in a sample.



Projection of atomic row tilted by 5 degrees seems a random atomic arrangement.

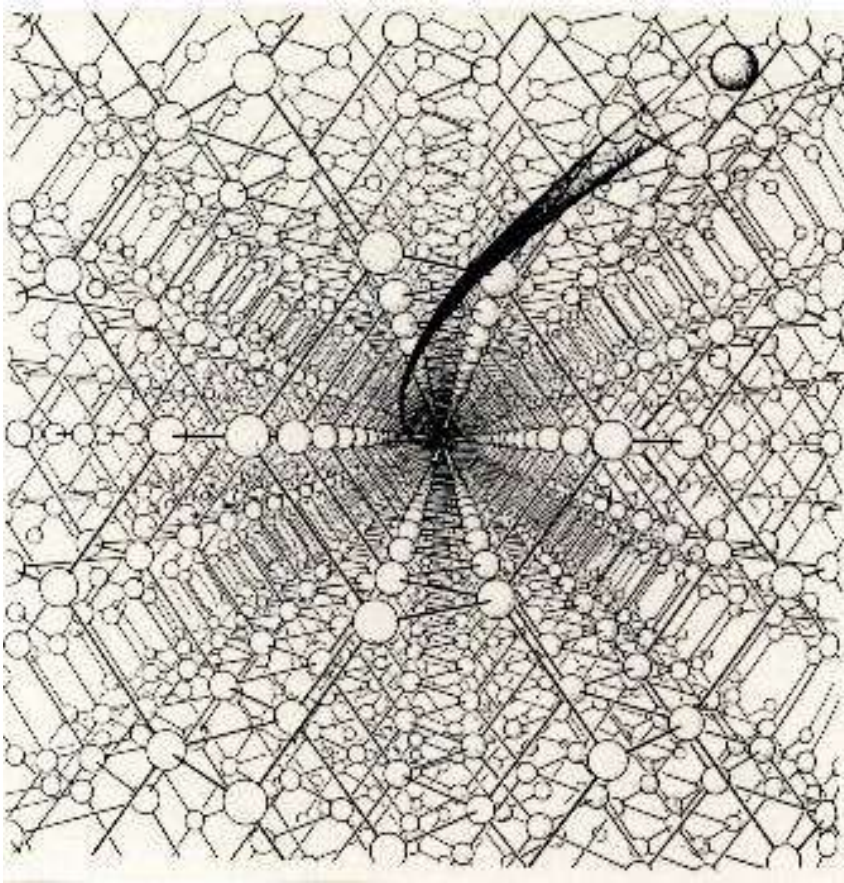
- **Channeling** gives information of amount and depth distribution of disorder, location of impurity in the lattice site, and composition and thickness of disordered surface layer.



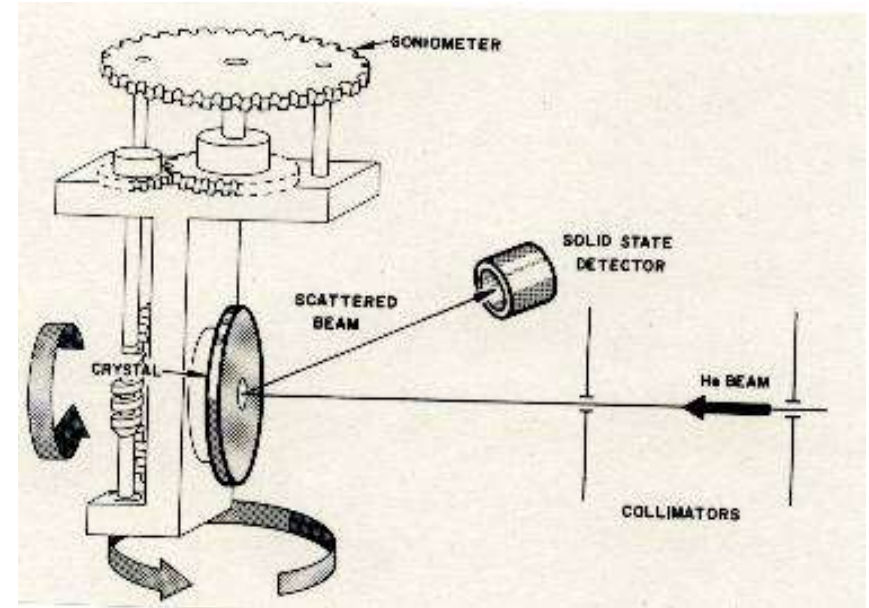
⊗ Ge<111> raw

*Wei-Kan Chu et al.,
Backscattering Spectrometry, AP*

Ion Channeling in crystal



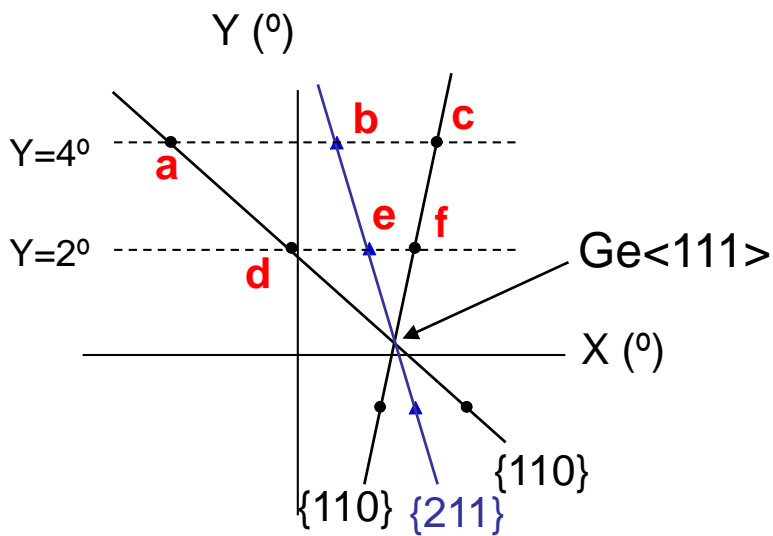
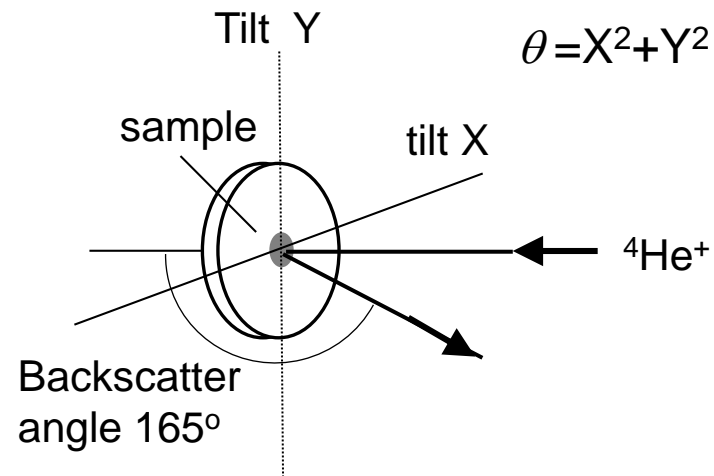
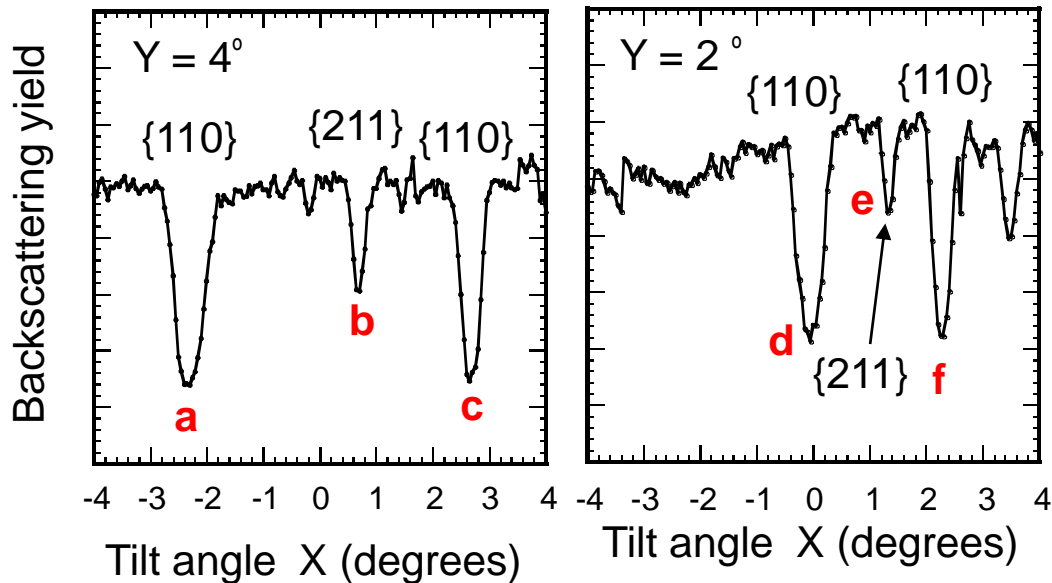
“Channeling in crystals”



L.C. Feldman, J. W. Mayer, S. T. Picraux, “Materials analysis by ion channeling”, Academic Press, 1982.

incident ions from a specific direction into crystals can travel inside of the crystal channel, so that backscattering yield and stopping power decreases drastically.

Alignment of crystal axis, Case of Ge<111>



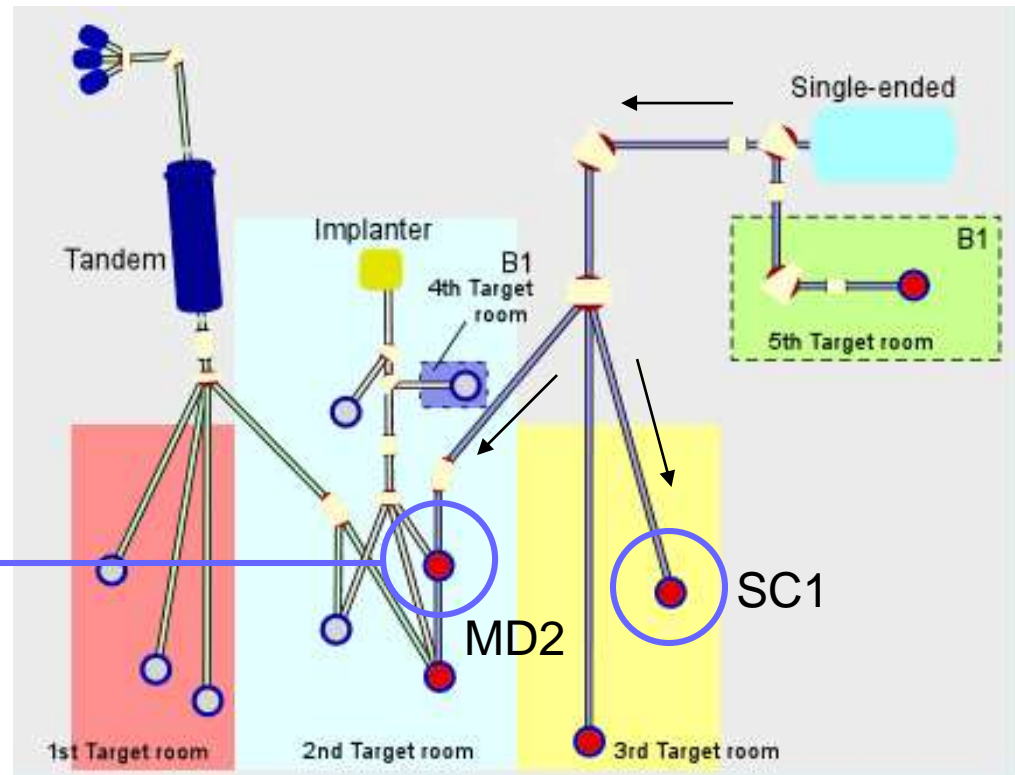
On Ge(111) plain, the zone axis of Ge<111> can be found by tilting along two specific direction, X and Y. This alignment of the axis controls accuracy of ion beam channeling.

RBS measurements at JAEA-TIARA

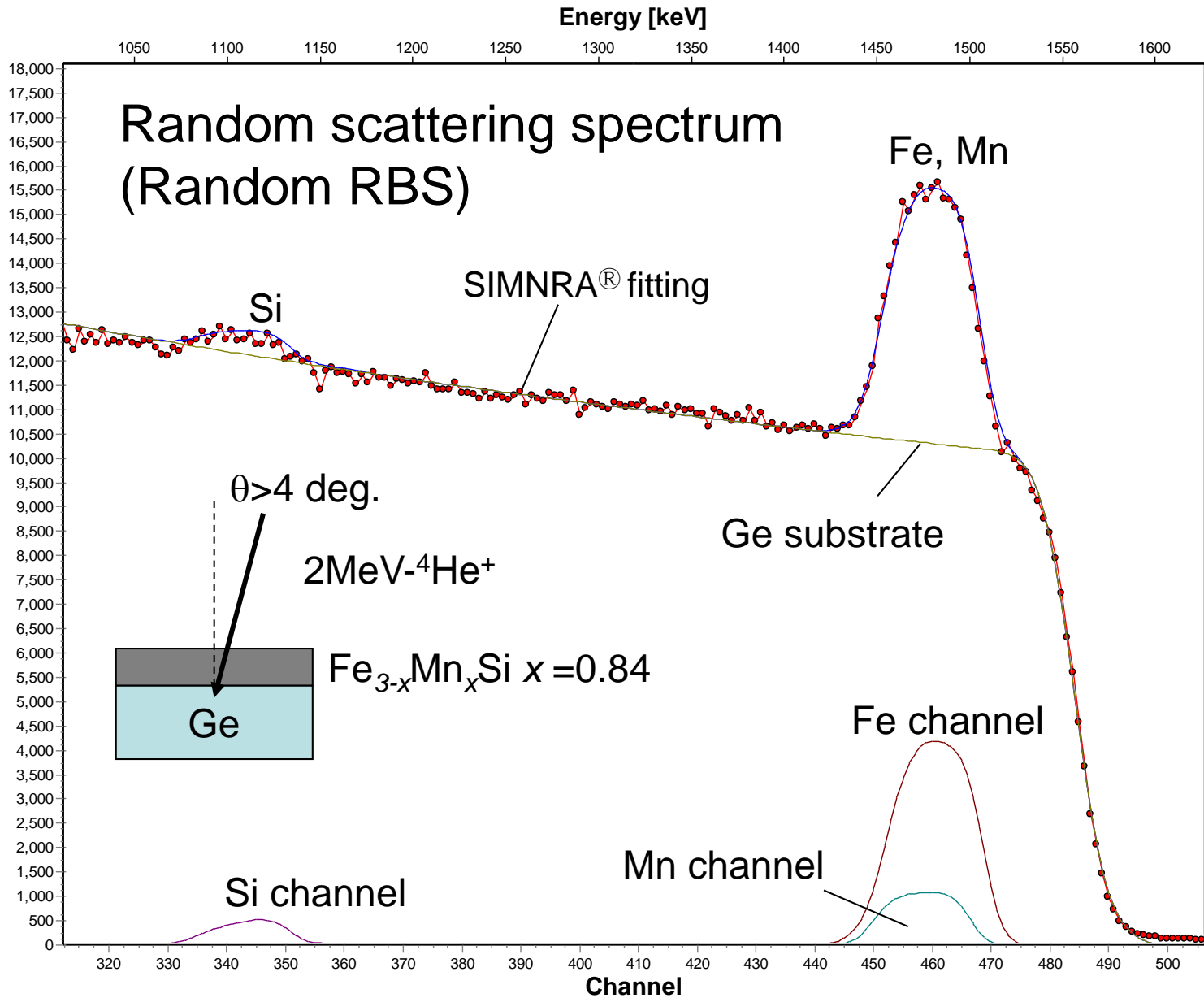
Dual Beam Analysis Line(MD2)
ion channeling set-up at low temperature



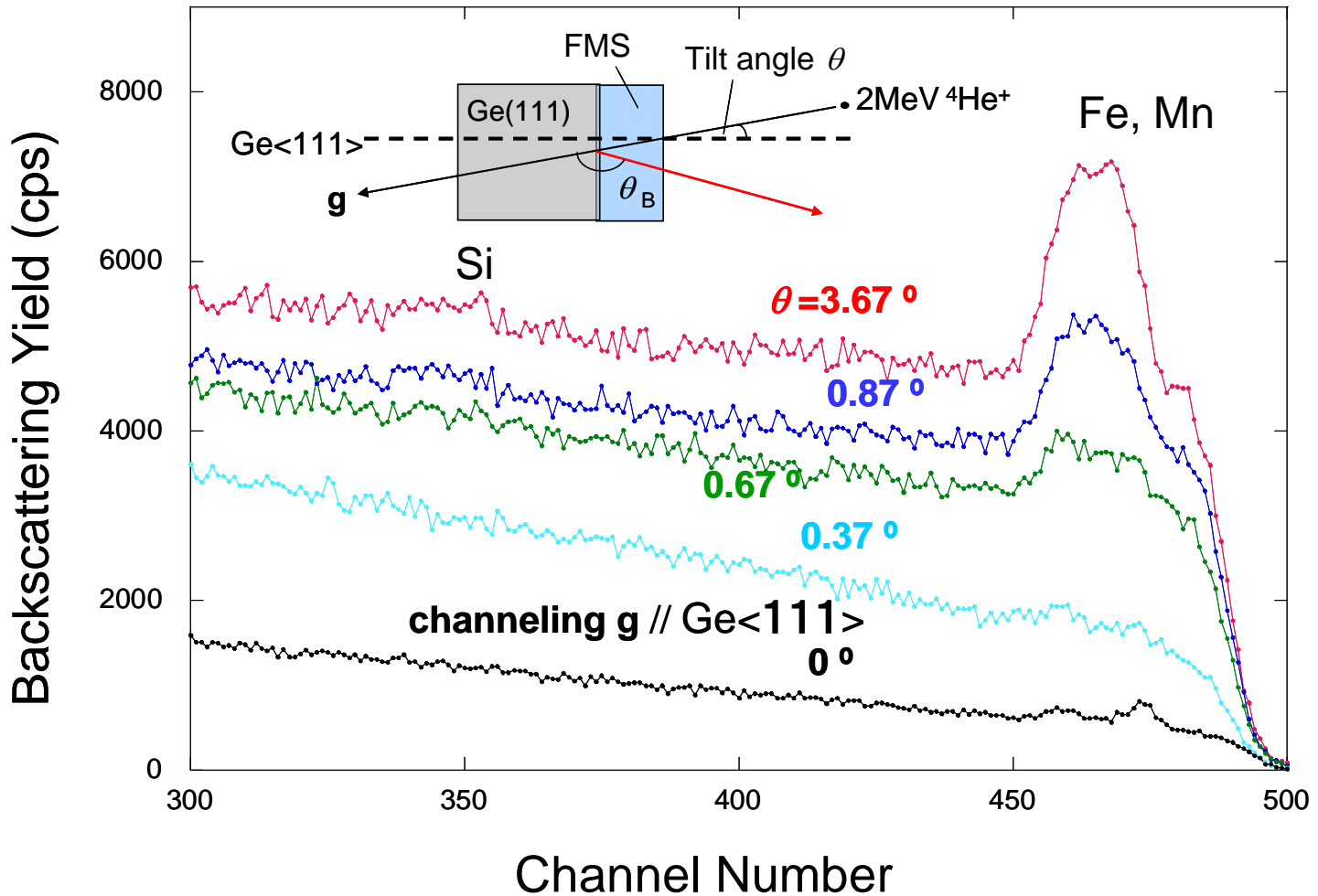
(Cited from Homepage of JAEA-TIARA)



Rutherford Backscattering (RBS)



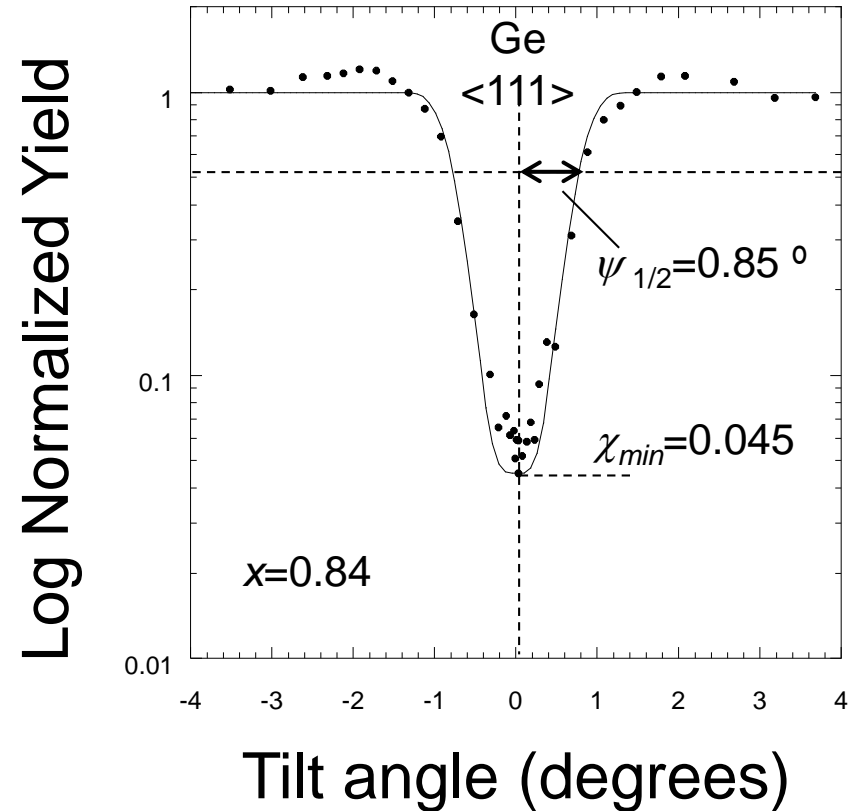
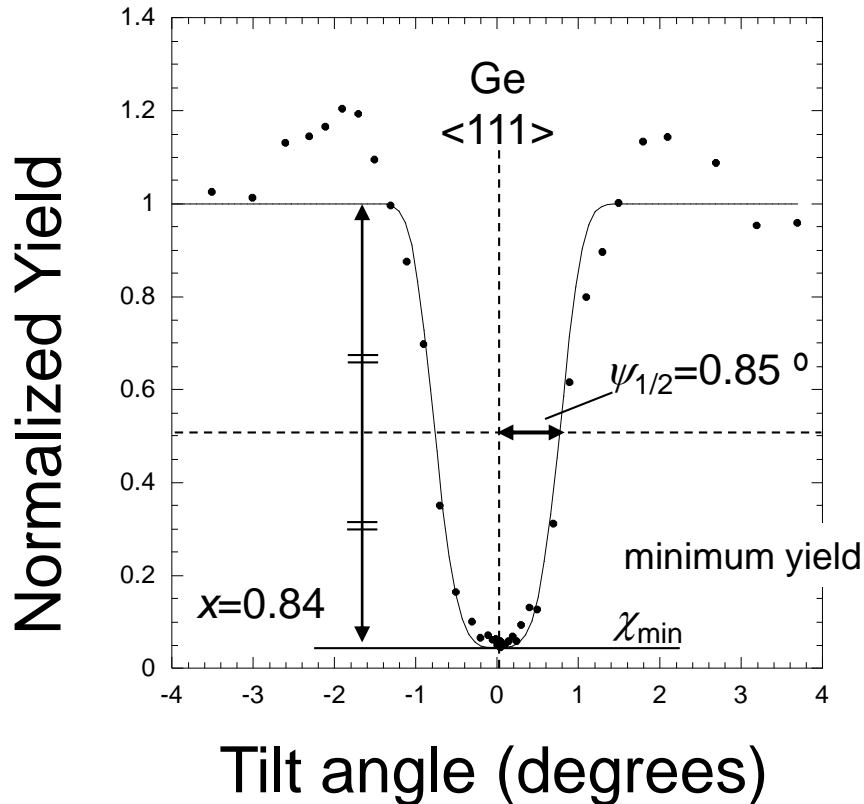
RBS measurements from aligned to random spectrum



When a sample is tilted from aligned angle, RBS spectrum changes continuously from channeling to random scattering.

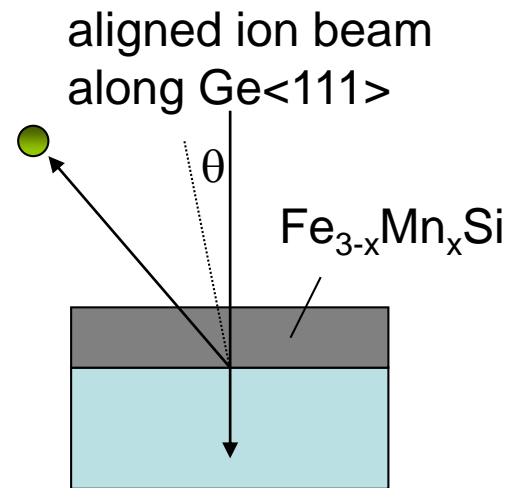
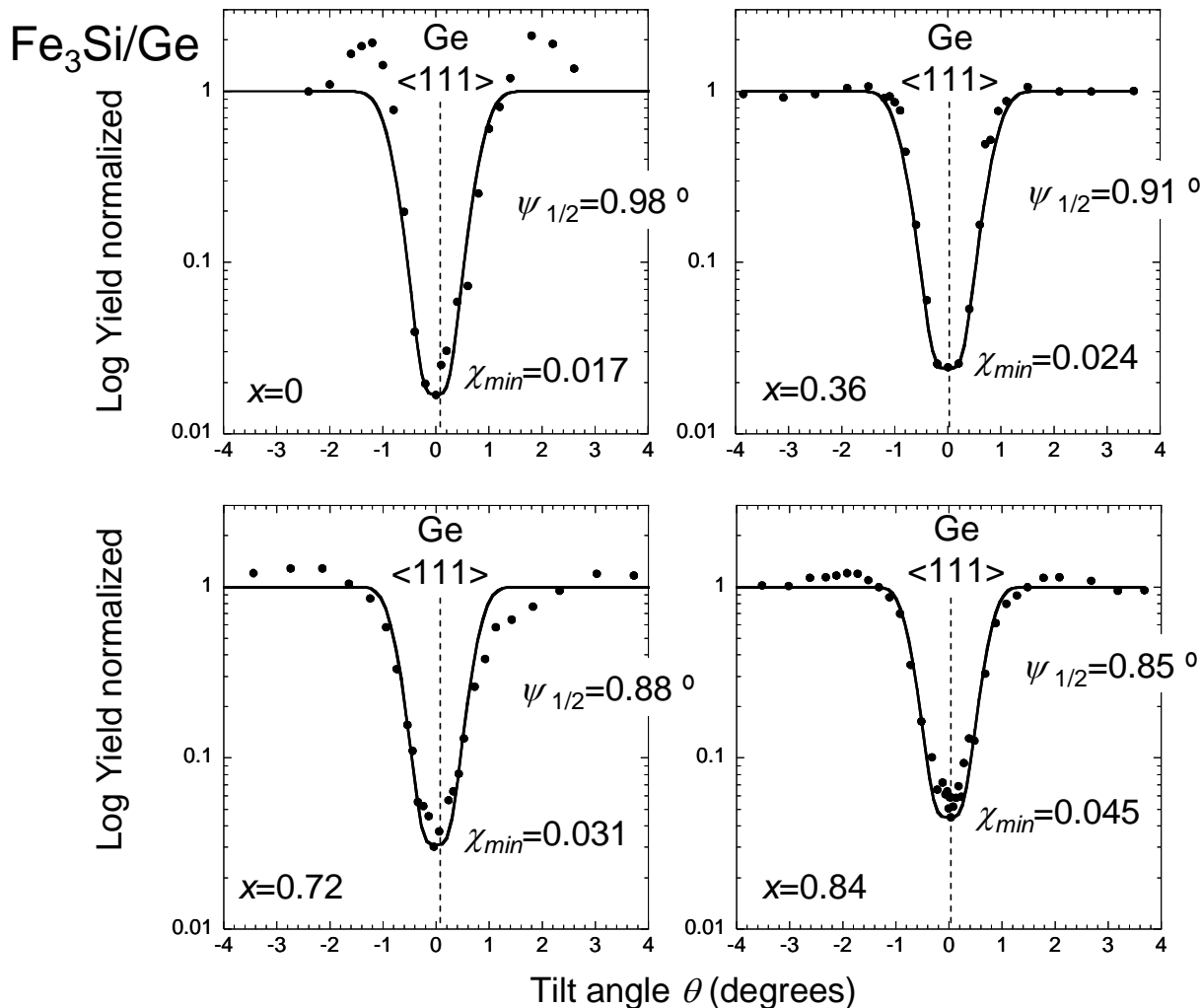
Angular yield profiles, Channeling parameter

$$\chi(\theta) = 1 - (1 - \chi_{\min}) \exp\left(-\ln 2 \left(\frac{\theta - \theta_0}{\psi_{1/2}}\right)^m\right)$$



Using the upper equation, deconvolution of angular yield profile for Fe and Mn can be performed and channeling parameter χ_{\min} and $\psi_{1/2}$ were obtained.

Fe_{3-x}Mn_xSi/Ge(111) hybrid structure at interfaces



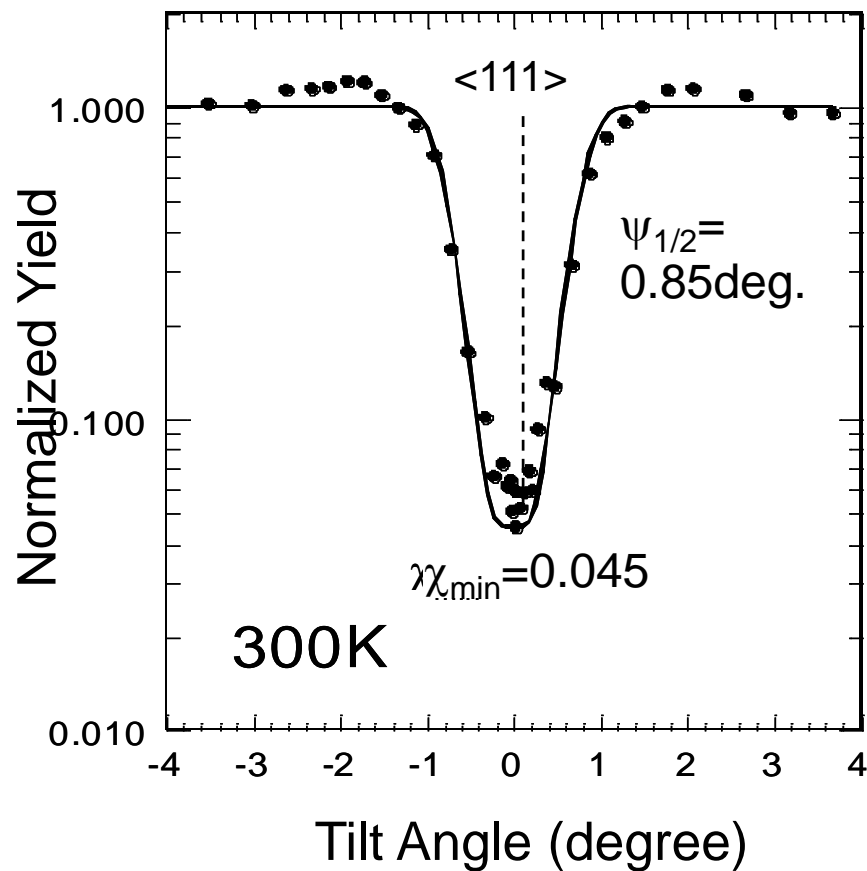
Resolution in depth
~2nm under geometric
condition employed.

We observed systematic increase of the minimum yield and decrease of the critical half angle as Mn content increased. All FMS with each Mn content maintained epitaxy with Ge(111).

Angular yield profiles at the interfaces with Ge(111)

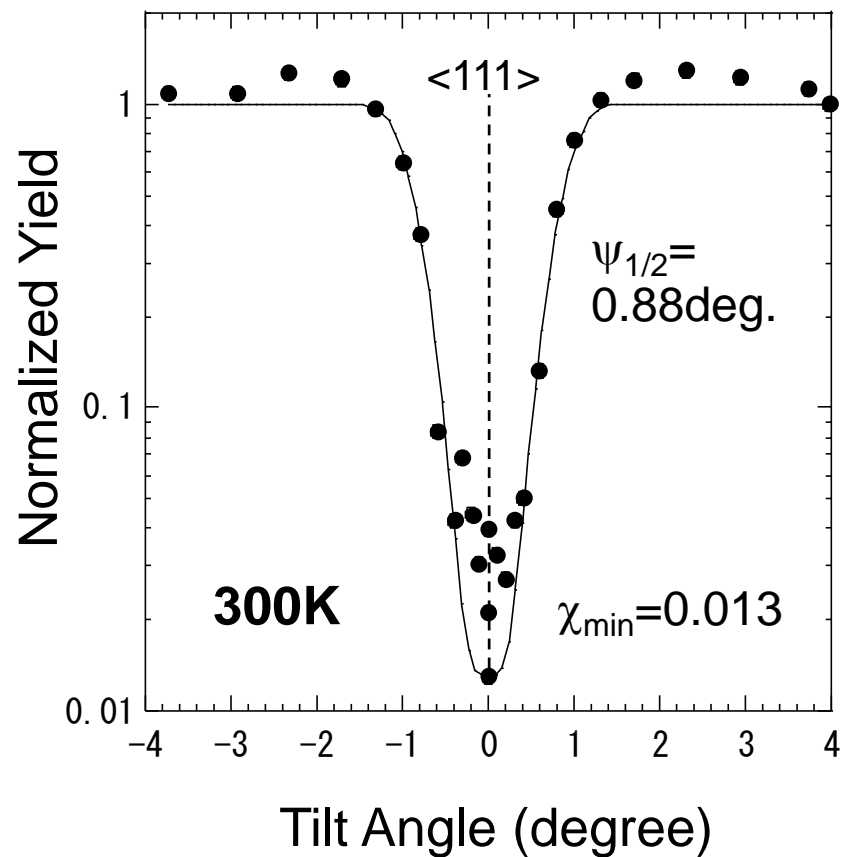
FMS/Ge

Fe₂MnSi/Ge(111)

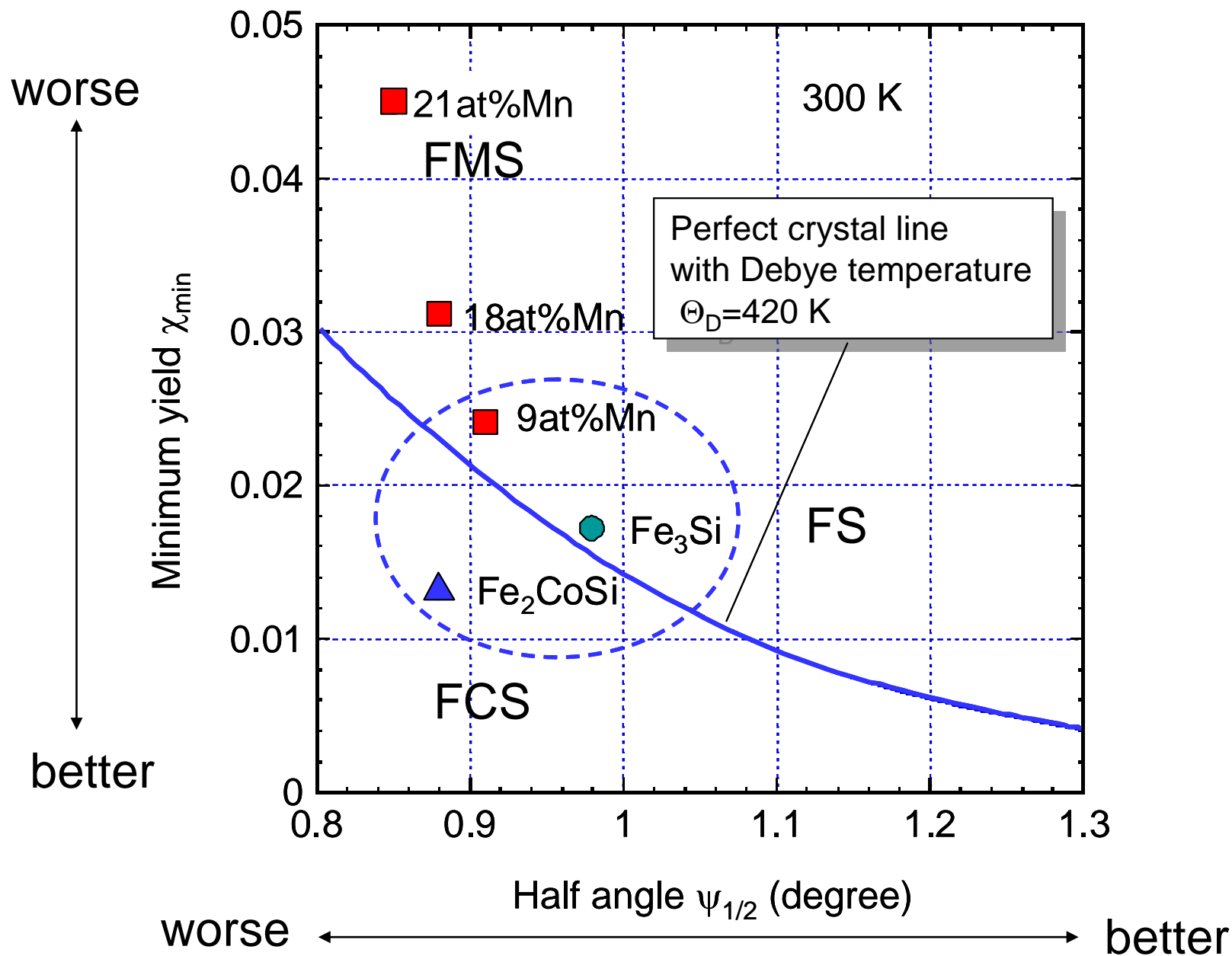


FCS/Ge

Fe₂CoSi/Ge(111)



Summary of results



Toward quantitative analysis using channeling parameter

Barrett-Gemmell model teaches us the way to quantitative analysis using channeling parameter (χ_{\min} , $\psi_{1/2}$).

$$\chi_{\min} = 18.8Nd \langle u \rangle^2 \sqrt{1 + \frac{1}{\zeta^2}}$$

$$\zeta = \frac{126 \langle u \rangle}{\psi_{1/2} d}$$

$\langle u \rangle$: total atomic displacement

N: atomic density

d: interatomic spacing in axial directions

Fortunately, we can solve above simultaneous equations using elementary mathematics.

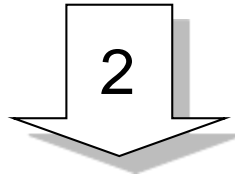
1

J. H. Barrett, *Phys. Rev. B* **3** (1971) 1527.

D. S. Gemmell, *Rev. Mod. Phys.* **46** (1974) 129.

How can we deduce $\langle u \rangle$ from channeling parameter?

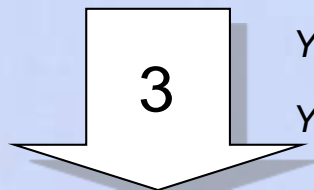
$(\chi_{\min}, \psi_{1/2})$ deduced from angular yield profile



$$A = \left(\frac{\psi_{1/2} d}{126} \right)^2, \quad B = \left(\frac{\chi_{\min}}{18.8Nd} \right)^2$$

$$\langle u \rangle (\text{\AA}) = \frac{1}{\sqrt{2}} \sqrt{\sqrt{A^2 + 4B} - A}$$

Remarks: under the condition at the same energy of incident ions



Y. Maeda et al.: *MRS Proc.* **1119E** (2008) 1119-L05-02.

Y. Maeda et al.: *Thin Solid Films* **519** (2011) 8461-8467.

Total atomic displacement along atomic row

Total displacement can be written by sum of contributions of thermal vibration and static displacement due to some imperfection in the atomic row.

$$\langle u \rangle^2 = \langle u_{th} \rangle^2 + \langle u_s \rangle^2$$

For perfect crystals or crystals with small imperfection being not detectable

$$\langle u \rangle^2 = \langle u_{th} \rangle^2$$

Calculation of $\langle u_{th} \rangle$

Debye model teaches us the one dimensional thermal vibration of a given atom, if the Debye temperature Θ_D of material is known.

Only for *i*-th element,

$$\langle u_{th} \rangle (\text{\AA}) = 12.1 \left[\left(\frac{\phi(y)}{y} + \frac{1}{4} \right) / \mu_i \Theta_D \right]^{1/2}$$

$$\phi(y) = \frac{1}{y} \int_0^y \frac{t}{e^t - 1} dt, \quad y = \frac{\Theta_D}{T} \quad \mu_i : \text{reduced mass}$$

5

First order Debye function

$$\phi(y) = \frac{1}{y} \int_0^y \frac{t}{e^t - 1} dt,$$

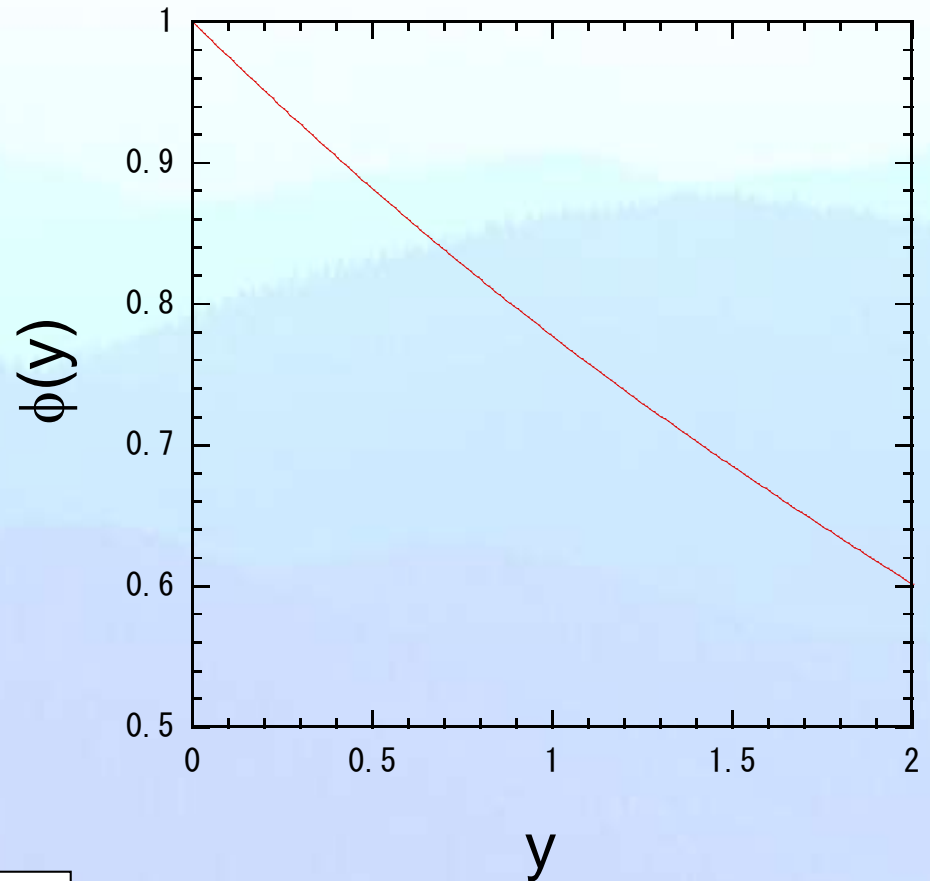
$$y = \frac{\Theta_D}{T}$$

Case of Fe₂MnSi

$\Theta_D = 420\text{K}$

$T = 300\text{K}$

$y = 1.4$



6

Calculation of static displacement $\langle u_s \rangle$ due to imperfection

$$(i) \langle u \rangle^2 \geq \langle u_{th} \rangle^2$$

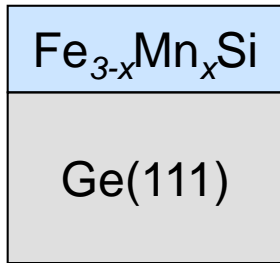
$$\langle u_s \rangle = \sqrt{\langle u \rangle^2 - \langle u_{th} \rangle^2}$$

$$(ii) \langle u \rangle^2 \leq \langle u_{th} \rangle^2$$

$$\langle u_s \rangle = \mathbf{0} \quad \text{corresponding to perfect crystals} \\ \text{or crystals with not detectable imperfection}$$

The static displacement can be obtained from subtraction between measured total displacement and calculated thermal vibration.

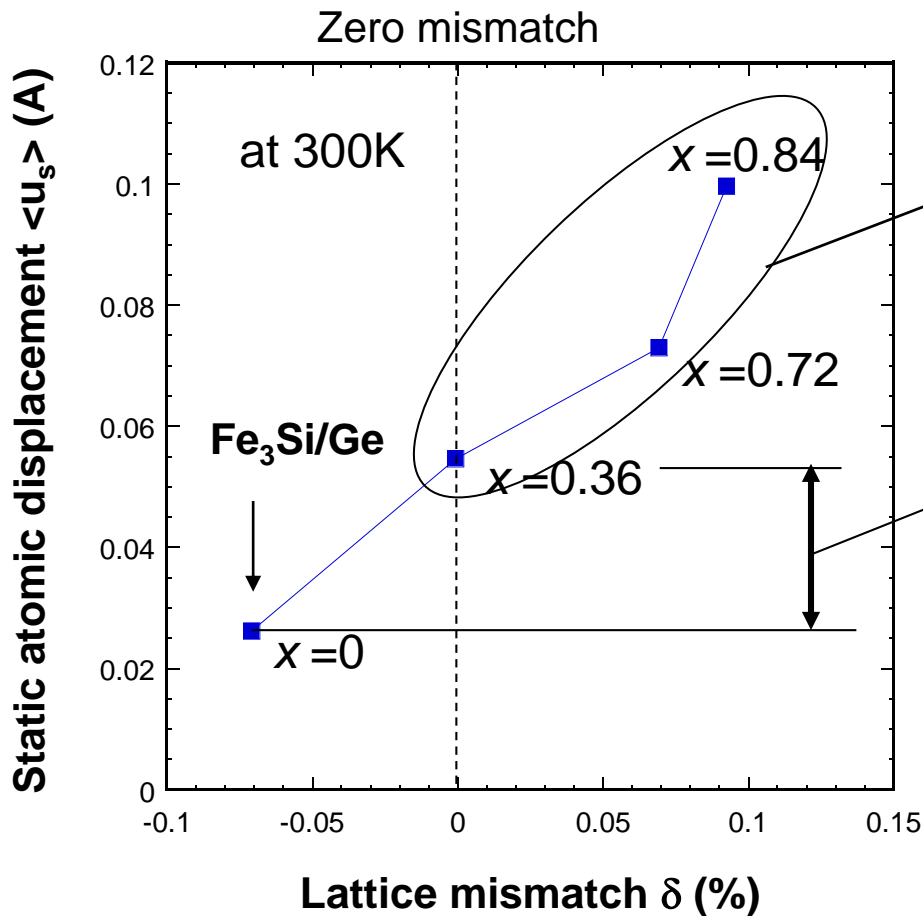
Static atomic displacement $\langle u_s \rangle$ at interface



$\delta(x)$ (%)

Lattice mismatch between FMS and Ge

$$\delta(x) = \left(\frac{(5.653 + 0.011x) - 5.657}{5.657} \right) \times 100$$



Strong correlation between $\langle u_s \rangle$ and lattice mismatch δ at the interface was found. This means that imperfection may mainly be introduced by the lattice mismatch.

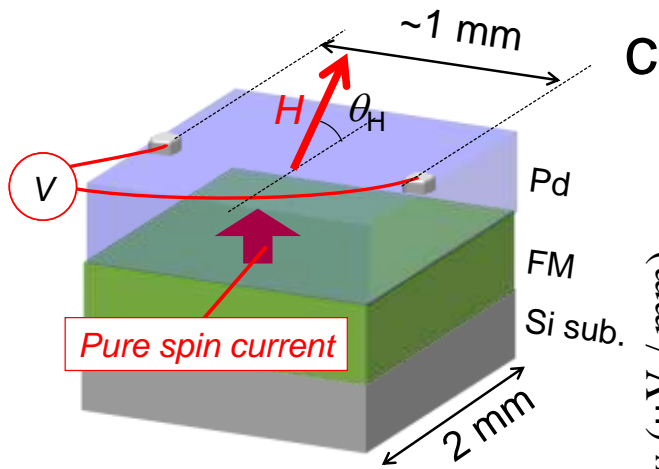
This difference may come from B site randomness due to Mn occupation.



Ferromagnetic resonance (FMR)

measurements

(Y. Andoh, APEC-SILICIDE 2013)



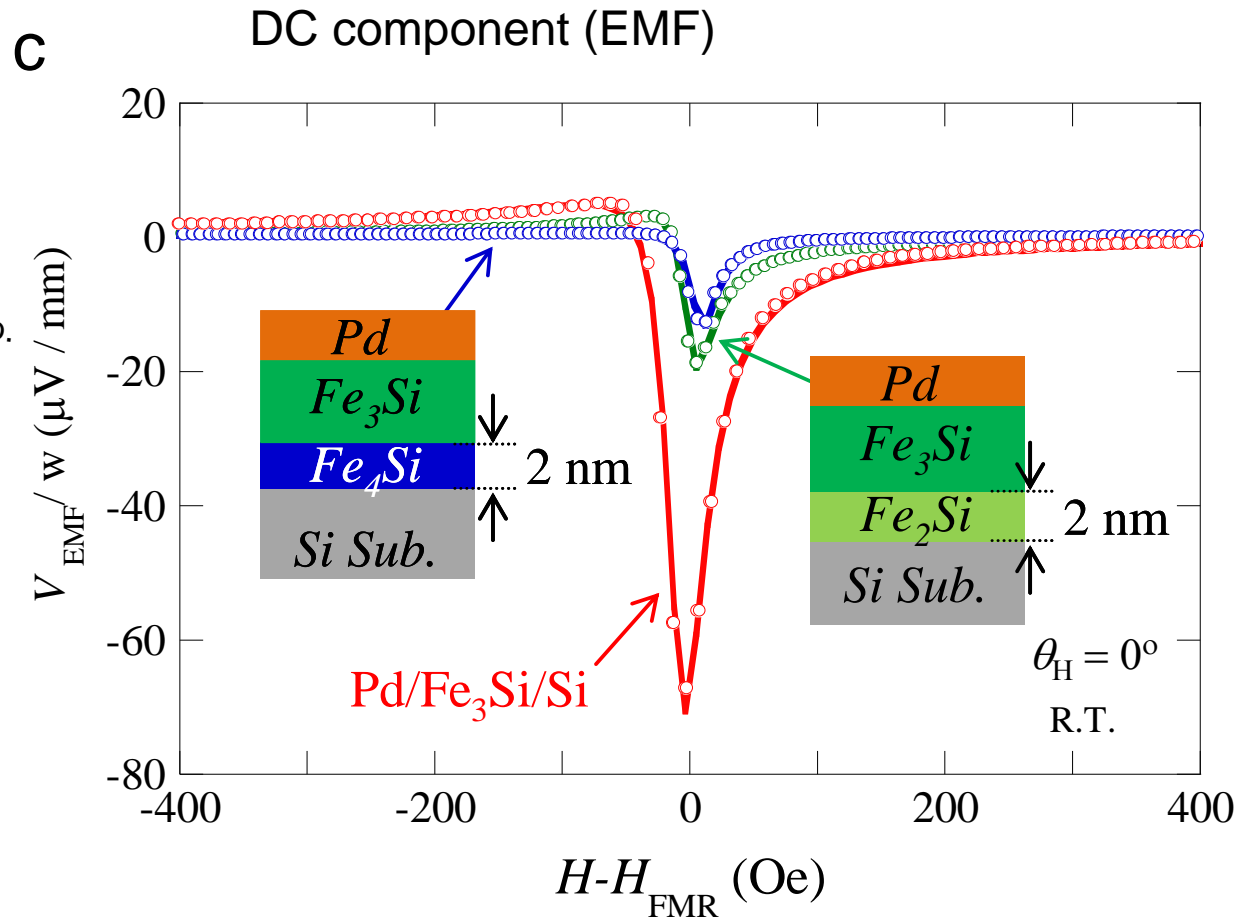
Measurements

ESR (Bruker EMX10/12)

Temp.: 300 K

Microwave power: 200 mW

Frequency: 9.6 GHz



These FMR measurements give the first confirmation that crystal quality of Fe₃Si directly controls performance of spin injection.

Conclusions

- Ion beam analysis (IBA) is helpful and powerful for analysis of epitaxial hetero-interfaces.
- It is possible to deduce quantitative and average information such as atomic displacements at a give depth or interface from the ion channeling parameter.
- Most recently, spin injection experiments are going more active. IBA data will be helpful for understanding its properties.

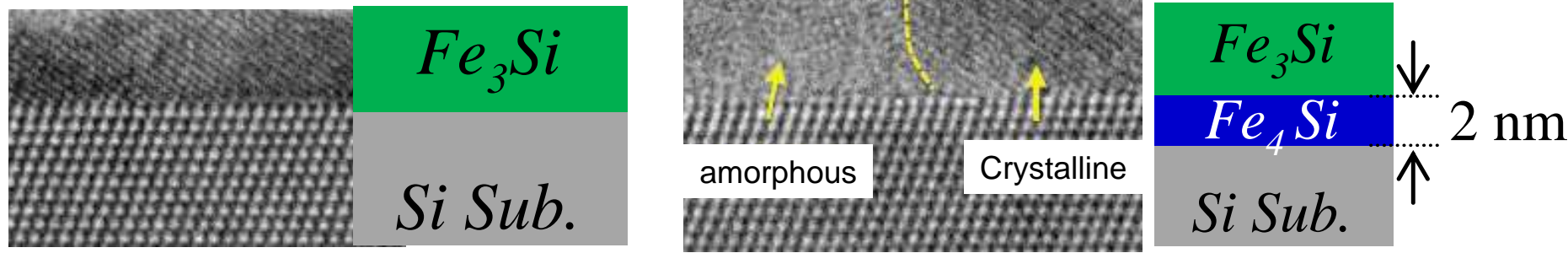




**Thank you for your kind
attention!**

Ion channeling of Fe_3Si , $Fe_4Si/Si(111)$

LTMBE



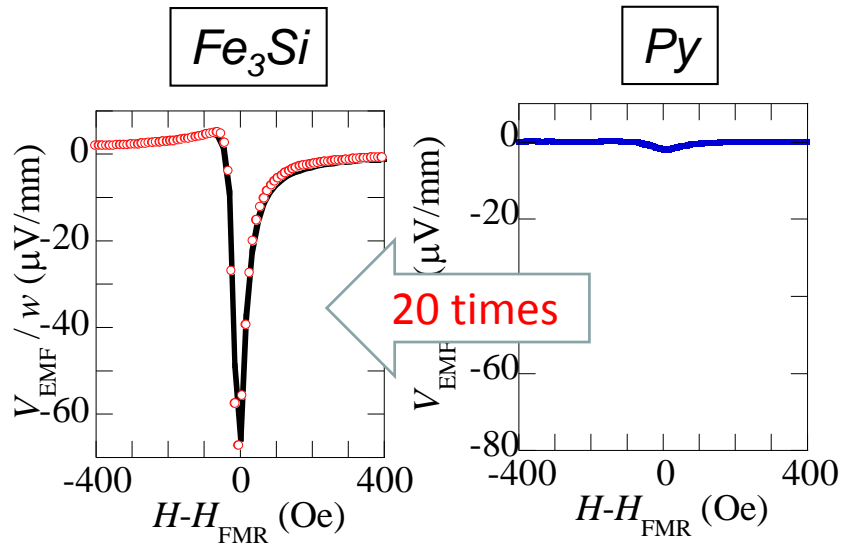
Results of ion channeling and static atomic displacement and spin injection experiment

	$\delta(\%)$ at IF	χ_{\min}	$\psi_{1/2}(\text{deg.})$	$\langle u_s \rangle (\text{\AA})$	emf (mV)
Fe_3Si/Si	+4.13	0.18	0.99	0.25	~68
Fe_4Si/Si	+4.15	0.23	0.95	0.52	~18
Fe_3Si/Ge	-0.05	0.02	0.98	0.09	

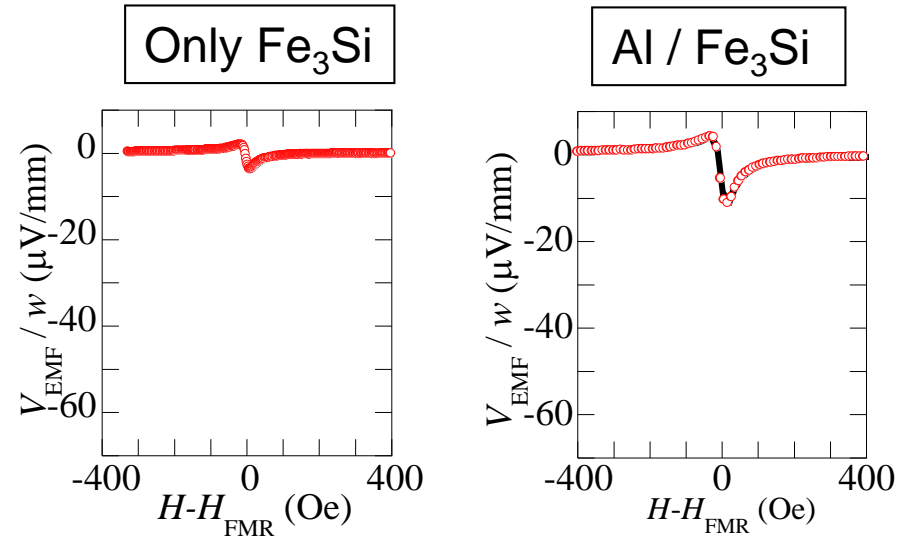
Dynamical spin injection into Pd layer using Fe₃Si

High quality Single crystalline Fe₃Si

① Large EMF



② Control experiments



To realize highly efficient generation of pure spin current...

✓ High quality FM layer with uniform magnetic properties.

✓ Small Gilbert damping constant

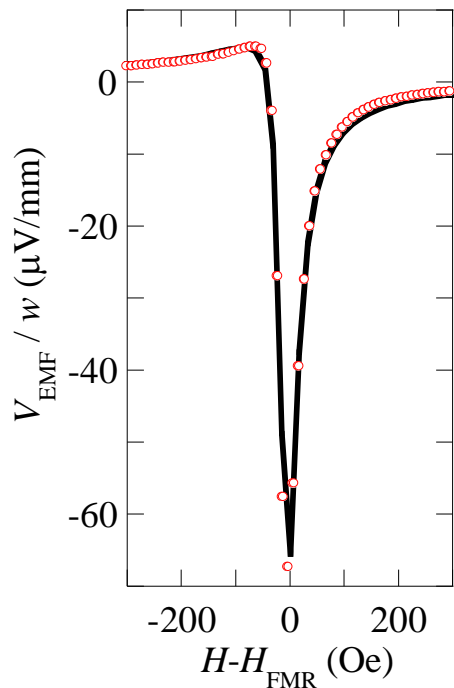
⇒ Ferromagnetic silicide Fe₃Si with homogeneous quality is promising.

(Y. Andoh, APEC-SILICIDE 2013)

Comparison of EMF for various FM samples

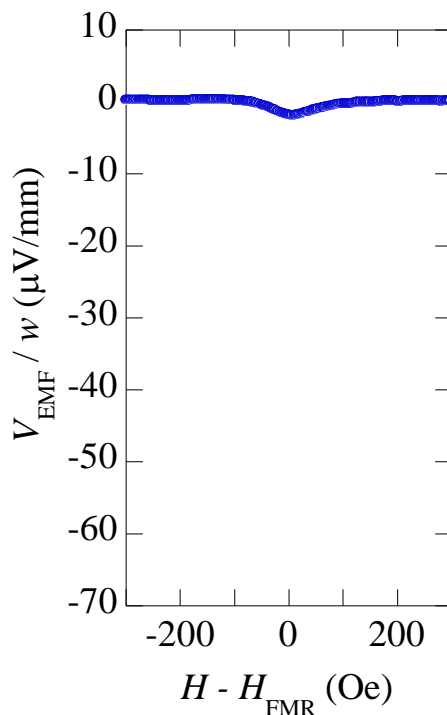
Single crystal

Pd/Fe₃Si



$$\frac{V_{\text{ISHE}}}{w} = 67.1 \mu\text{V}/\text{mm}$$

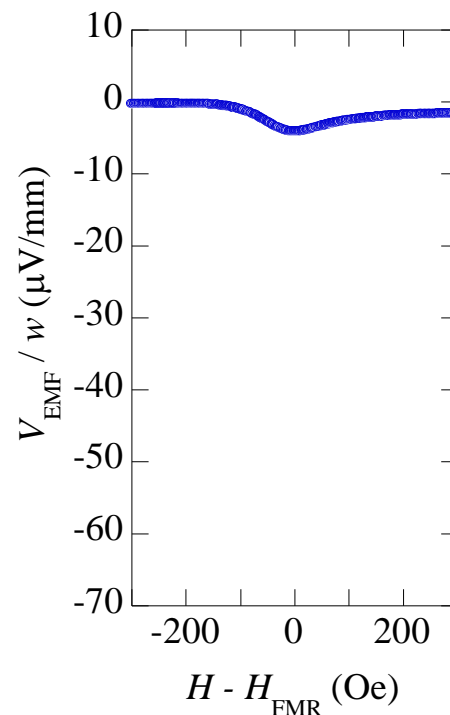
Pd/Py



$$\frac{V_{\text{ISHE}}}{w} = 3.05 \mu\text{V}/\text{mm}$$

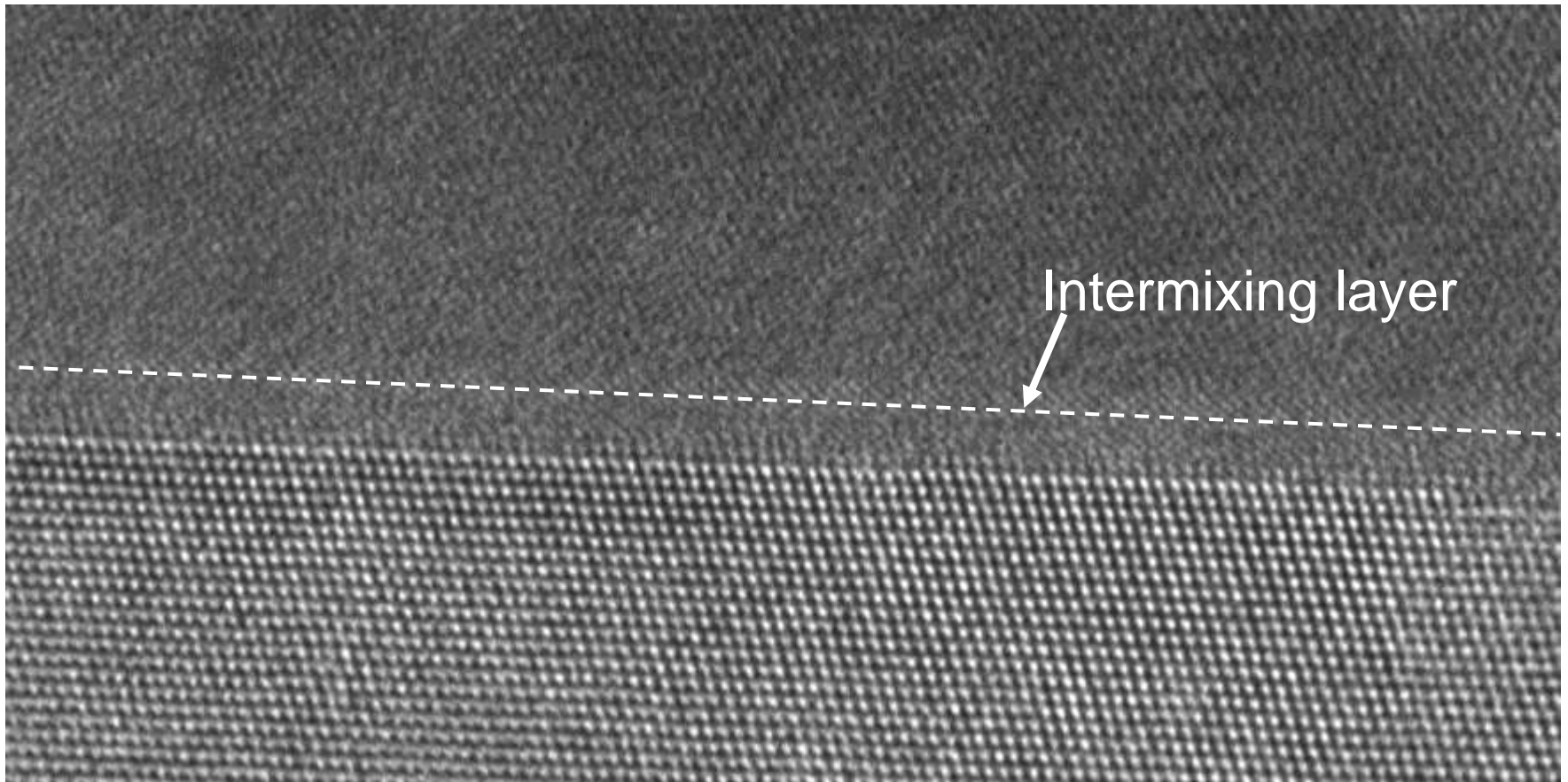
Single crystal

Pd/Co₆Fe₄



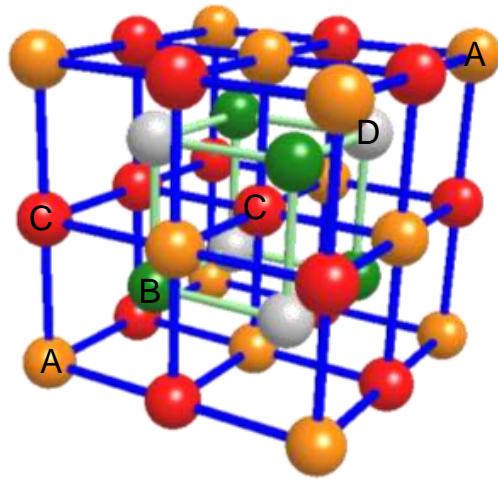
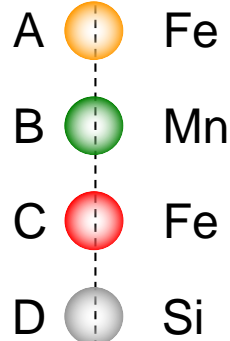
$$\frac{V_{\text{ISHE}}}{w} = 2.92 \mu\text{V}/\text{mm}$$

$\text{Fe}_2\text{MnSi}(111)/\text{Ge}(111)$ $T_d=200^\circ\text{C}$

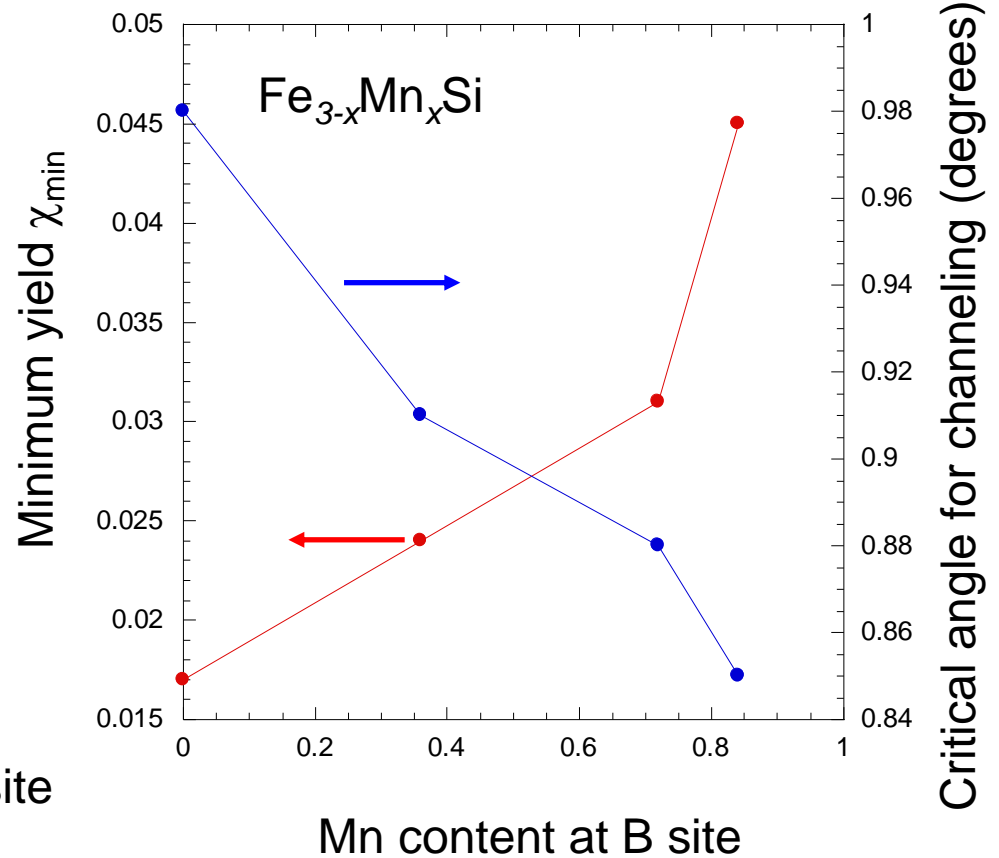


Axial channeling parameter (χ_{\min} , $\psi_{1/2}$)

$\langle 111 \rangle$



NMR and Moessbauer measurements revealed that in every Mn content, Mn atoms preferably occupy at the B site in the lattice.



We found that increase of Mn content at the B site brings randomness of the atomic row along $\langle 111 \rangle$ direction. This behavior has been observed as increase of a Debye-Waller factor in EXAF, XANES measurements. Randomness along $\langle 111 \rangle$ may be introduced by weak chemical bonds around Mn atoms at the B site.